

=> fil reg; d que 16; d stat que 132; fil capl; s 16 or 132
FILE=REGISTRY" ENTERED AT 14:10:25 ON 13 MAR 2002
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STRUCTURE FILE UPDATES: 11 MAR 2002 HIGHEST RN 400601-79-8
 DICTIONARY FILE UPDATES: 11 MAR 2002 HIGHEST RN 400601-79-8

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

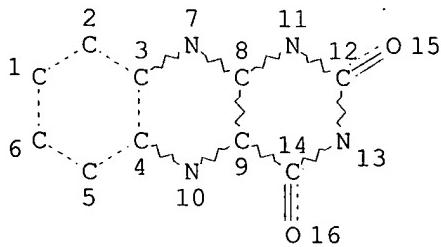
L5 49 SEA FILE=REGISTRY ABB=ON (9001-91-6/BI OR 109319-16-6/BI OR
 121-79-9/BI OR 128-37-0/BI OR 1953-02-2/BI OR 25013-16-5/BI OR
 3483-12-3/BI OR 50-81-7/BI OR 50-99-7/BI OR 52-90-4/BI OR
 53188-07-1/BI OR 56-45-1/BI OR 56-81-5/BI OR 56-87-1/BI OR
 60-18-4/BI OR 63-68-3/BI OR 69-65-8/BI OR 70-18-8/BI OR
 71-00-1/BI OR 73-22-3/BI OR 73-24-5/BI OR 9000-94-6/BI OR
 9001-26-7/BI OR 9001-28-9/BI OR 9001-29-0/BI OR 9001-30-3/BI
 OR 9002-01-1/BI OR 9002-72-6/BI OR 9013-55-2/BI OR 9031-37-2/BI
 OR 9035-81-8/BI OR 9038-70-4/BI OR 9055-02-1/BI OR 98-92-0/BI
 OR 101750-71-4/BI OR 113189-02-9/BI OR 28083-73-0/BI OR
 335333-92-1/BI OR 335333-93-2/BI OR 335333-94-3/BI OR 335333-95
 -4/BI OR 335333-96-5/BI OR 362467-62-7/BI OR 362467-63-8/BI OR
 362467-64-9/BI OR 3942-96-9/BI OR 47061-66-5/BI OR 616-91-1/BI
 OR 9001-27-8/BI)

~~FILE~~ 12 SEA FILE=REGISTRY ABB=ON L5 AND NR>2

*structures
from applicants' work*

L11

STR



*full file search
done on this structure*

NODE ATTRIBUTES:

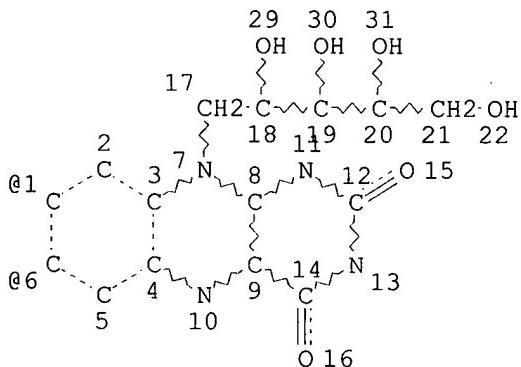
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L13 4344 SEA FILE=REGISTRY SSS FUL L11
L19 STR



*subset search done
looking for this
structure
(p. 54)*

Me @23 25 27
24 Ak ~ N @26 28

VPA 23-1/6 U
VPA 26-1/6 U

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 25
CONNECT IS E2 RC AT 27
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

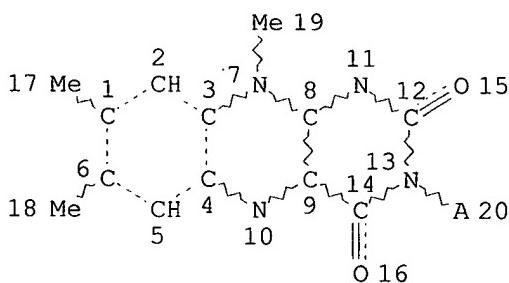
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

or this structure

(elm 59)



NODE ATTRIBUTES:

NSPEC IS RC AT 20
 CONNECT IS E3 RC AT 3
 CONNECT IS E3 RC AT 4
 CONNECT IS E3 RC AT 8
 CONNECT IS E3 RC AT 9
 CONNECT IS E2 RC AT 10
 CONNECT IS E2 RC AT 11
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

all the compounds here have

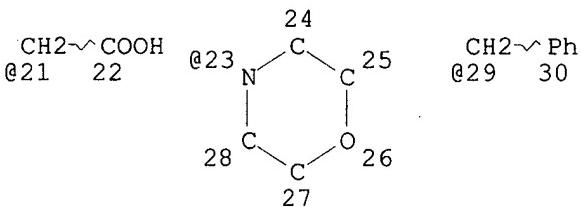
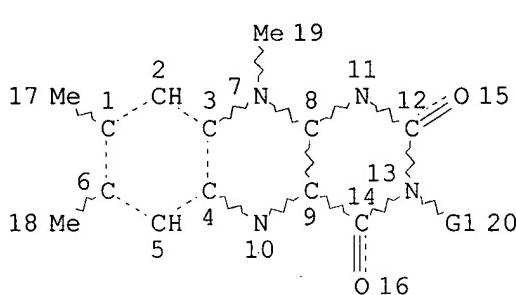
R₁, R₂, R₃ Me.

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L26 76 SEA FILE=REGISTRY SUB=L13 SSS FUL (L19 OR L24)
 L30 STR



*this structure "not"-ed out of
 answer set (addresses multiple provisions)*

CH2~CH2~NH
 @31 32 33

VAR G1=31/23/ME/21/29

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 3
 CONNECT IS E3 RC AT 4
 CONNECT IS E3 RC AT 8
 CONNECT IS E3 RC AT 9
 CONNECT IS E2 RC AT 10
 CONNECT IS E2 RC AT 11
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 33

STEREO ATTRIBUTES: NONE

~~L32~~ 76 SEA FILE=REGISTRY SUB=L26 SSS FUL (L11 NOT L30)

100.0% PROCESSED 76 ITERATIONS
 SEARCH TIME: 00.00.01

~~743~~ ANSWERS

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FILE COVERS 1907 - 13 Mar 2002 VOL 136 ISS 11
FILE LAST UPDATED: 11 Mar 2002 (20020311/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

14 L6
59 L32
*L34 70 L6 OR L32

=> fil uspatf; s 16 or 132
FILE 'USPATFULL' ENTERED AT 14:10:50 ON 13 MAR 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 12 Mar 2002 (20020312/PD)
FILE LAST UPDATED: 12 Mar 2002 (20020312/ED)
HIGHEST GRANTED PATENT NUMBER: US6357047
HIGHEST APPLICATION PUBLICATION NUMBER: US2002029398
CA INDEXING IS CURRENT THROUGH 12 Mar 2002 (20020312/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 12 Mar 2002 (20020312/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2001
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2001

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<

>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
 >>> enter this cluster. <<<
 >>> <<<
 >>> Use USPATALL when searching terms such as patent assignees, <<<
 >>> classifications, or claims, that may potentially change from <<<
 >>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

2 L6
 2 L32
 L35
 2 L6 OR L32

=> dup rem 134,135
 FILE 'CAPLUS' ENTERED AT 14:11:32 ON 13 MAR 2002
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FILE 'USPATFULL' ENTERED AT 14:11:32 ON 13 MAR 2002
 CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)
 PROCESSING COMPLETED FOR L34
 PROCESSING COMPLETED FOR L35
 L37 72 DUP REM L34 L35 (0 DUPLICATES REMOVED)
 ANSWERS '1-70' FROM FILE CAPLUS
 ANSWERS '71-72' FROM FILE USPATFULL

=> d ibib abs hitstr 137 1-72; fil caol; d que nos 136

L37 ANSWER 1 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:300555 CAPLUS
 DOCUMENT NUMBER: 134:316078
 TITLE: Isoalloxazine derivatives to neutralize biological contaminants
 INVENTOR(S): Platz, Matthew Stewart; Goodrich, Raymond Paul, Jr.
 PATENT ASSIGNEE(S): Gambio, Inc., USA
 SOURCE: PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001028599	A1	20010426	WO 2000-US25213	20000915
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6268120	B1	20010731	US 1999-420652	19991019

PRIORITY APPLN. INFO.: US 1999-420652 A 19991019

OTHER SOURCE(S): MARPAT 134:316078

AB Methods are provided for neutralization of microorganisms in fluids or on surfaces. Preferably the fluids contain blood or blood products and

comprise biol. active proteins. Preferred methods include the steps of adding an activation-effective amt. of a microorganism neutralizer with an isoalloxazine backbone to a fluid and exposing the fluid to a triggering event. Preferred triggering events include light of a suitable wavelength and intensity to activate the microorganism neutralizer or a pH sufficient to activate the microorganism neutralizer. Other fluids, including juices, water and the like, may also be decontaminated by these methods as may surfaces of foods, animal carcasses, wounds, food prepn. surfaces and bathing and washing vessel surfaces. Compds. with an isoalloxazine backbone are also provided. For example, neutralization of microorganisms in blood with 7,8,10-trimethyl,3-sulfonylisoalloxazine (10 .mu.M) and light irradn. was carried out.

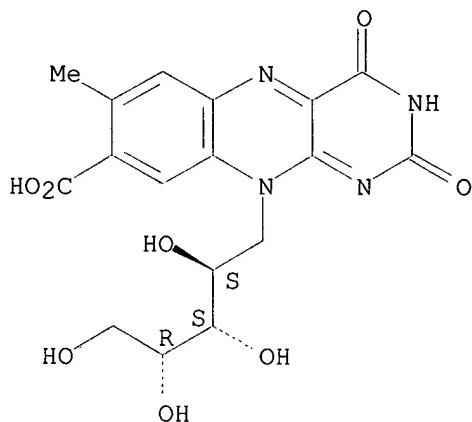
IT 28083-73-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(neutralization of biol. contaminants by isoalloxazine derivs.)

RN 28083-73-0 CAPLUS

CN Riboflavin, 8-carboxy-8-demethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

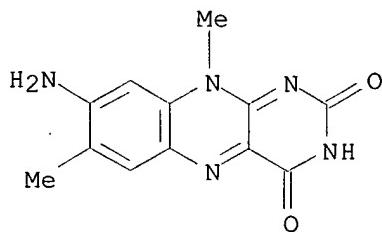


IT 3942-96-9P 101750-71-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(neutralization of biol. contaminants by isoalloxazine derivs.)

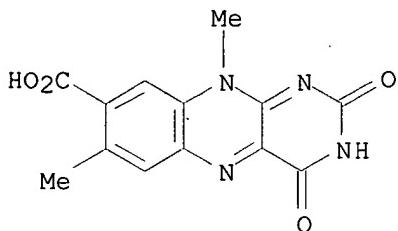
RN 3942-96-9 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



RN 101750-71-4 CAPLUS

CN Benzo[g]pteridine-8-carboxylic acid, 2,3,4,10-tetrahydro-7,10-dimethyl-2,4-dioxo- (6CI, 9CI) (CA INDEX NAME)



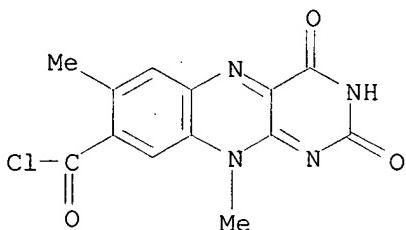
IT 335333-92-1P 335333-93-2P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(neutralization of biol. contaminants by isoalloxazine derivs.)

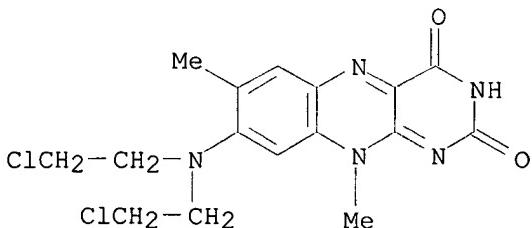
RN 335333-92-1 CAPLUS

CN Benzo[g]pteridine-8-carbonyl chloride, 2,3,4,10-tetrahydro-7,10-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



RN 335333-93-2 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-[bis(2-chloroethyl)amino]-7,10-dimethyl- (9CI) (CA INDEX NAME)



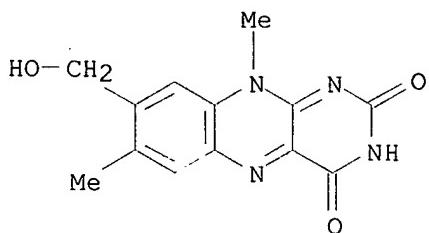
IT 47061-66-5 335333-94-3 335333-95-4

335333-96-5

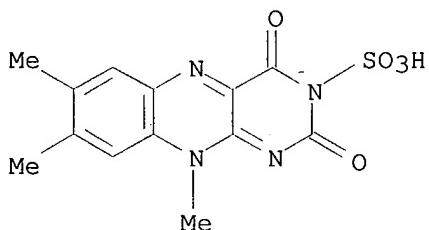
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(neutralization of biol. contaminants by isoalloxazine derivs.)

RN 47061-66-5 CAPLUS

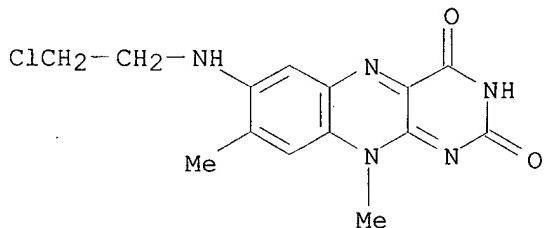
CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-(hydroxymethyl)-7,10-dimethyl- (9CI) (CA INDEX NAME)



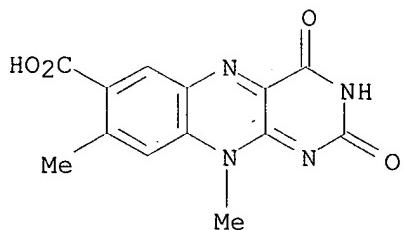
RN 335333-94-3 CAPLUS
 CN Benzo[g]pteridine-3(2H)-sulfonic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



RN 335333-95-4 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7-[(2-chloroethyl)amino]-8,10-dimethyl- (9CI) (CA INDEX NAME)



RN 335333-96-5 CAPLUS
 CN Benzo[g]pteridine-7-carboxylic acid, 2,3,4,10-tetrahydro-8,10-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 2 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:713845 CAPLUS
 DOCUMENT NUMBER: 135:251944
 TITLE: Isoalloxazine derivatives to neutralize biological

INVENTOR(S): contaminants
 Platz, Matthew Stewart; Goodrich, Raymond Paul
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 22 pp., Cont.-in-part of U.S.
 6,268,120.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 2001024781	A1	20010927	US 2001-777727	20010205
US 6268120	B1	20010731	US 1999-420652	19991019

PRIORITY APPLN. INFO.: US 1999-420652 A2 19991019

OTHER SOURCE(S): MARPAT 135:251944

AB Methods are provided for neutralization of microorganisms in fluids or on surfaces. Preferably the fluids contain blood or blood products and comprise biol. active proteins. Preferred methods include the steps of adding an activation-effective amt. of a microorganism neutralizer with an isoalloxazine backbone to a fluid and exposing the fluid to a triggering event. Preferred triggering events include light of a suitable wavelength and intensity to activate the microorganism neutralizer or a pH sufficient to activate the microorganism neutralizer. Other fluids, including juices, water and the like, may also be decontaminated by these methods as may surfaces of foods, animal carcasses, wounds, food prepn. surfaces and bathing and washing vessel surfaces. Compds. with an isoalloxazine backbone are also provided.

IT 362467-62-7 362467-63-8 362467-64-9

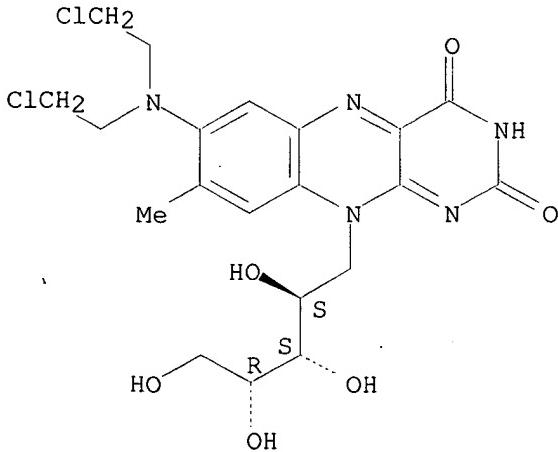
RL: BAC (Biological activity or effector, except adverse); BUU (Biological use, unclassified); FFD (Food or feed use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(isoalloxazine derivs. to neutralize biol. microorganism contaminants in fluids or on surfaces in relation to activation by light or pH)

RN 362467-62-7 CAPPLUS

CN D-Ribitol, 1-[7-[bis(2-chloroethyl)amino]-3,4-dihydro-8-methyl-2,4-dioxobenzo[g]pteridin-10(2H)-yl]-1-deoxy- (9CI) (CA INDEX NAME)

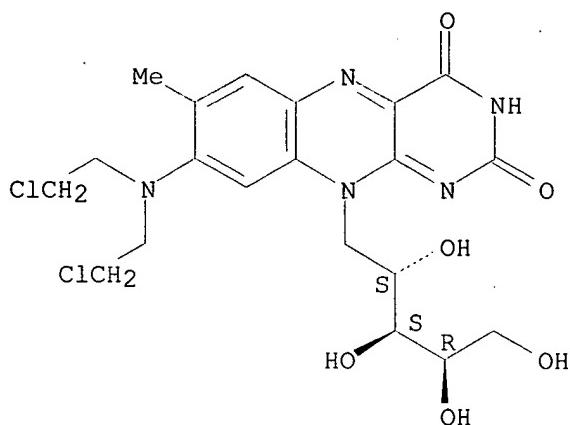
Absolute stereochemistry.



RN 362467-63-8 CAPPLUS

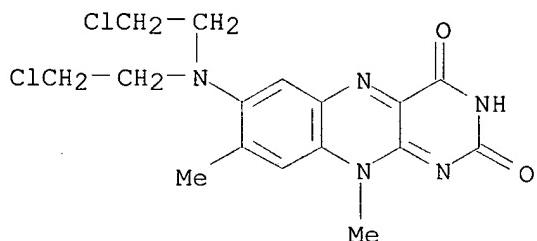
CN D-Ribitol, 1-[8-[bis(2-chloroethyl)amino]-3,4-dihydro-7-methyl-2,4-dioxobenzo[g]pteridin-10(2H)-yl]-1-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 362467-64-9 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7-[bis(2-chloroethyl)amino]-8,10-dimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 3 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:207004 CAPLUS

DOCUMENT NUMBER: 135:5794

TITLE: Synthesis and characterization of flavin-tethered peptide nucleic acid

AUTHOR(S): Ikeda, Hisafumi; Yoshida, Kohzo; Ozeki, Makoto; Saito, Isao

CORPORATE SOURCE: Faculty of Engineering, Department of Synthetic Chemistry and Biological Chemistry, Japan Science and Technology Corporation, CREST, Kyoto University, Yoshida, Sakyo, Kyoto, 606-8501, Japan

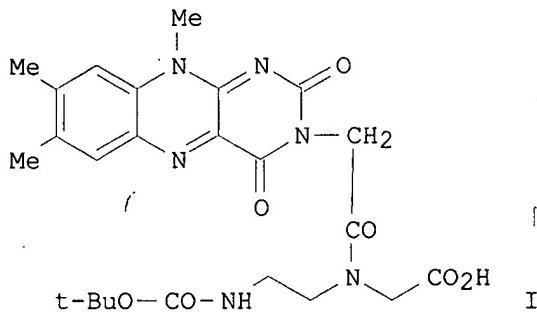
SOURCE: Tetrahedron Letters (2001), 42(13), 2529-2531

PUBLISHER: CODEN: TELEAY; ISSN: 0040-4039 Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



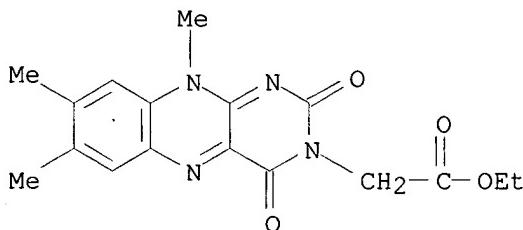
AB We synthesized flavin-contg. PNA monomer unit (I) from lumiflavin and prep'd. PNAs contg. a flavin moiety (FPNA) by the std. tBoc chem. Each PNA oligomer was purified by reversed-phase HPLC and characterized by MALDI-TOF MS and UV spectra. Thermodn. analyses indicated that the PNA oligomer contg. a flavin moiety near the amino terminal considerably stabilized the PNA-DNA hybrids.

IT 74178-39-5P 340259-04-3P 340259-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and characterization of flavin-tethered peptide nucleic acid
for use in PNA-DNA hybrids)

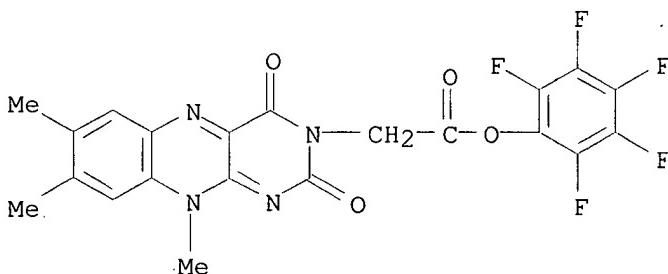
RN 74178-39-5 CAPPLUS

CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (7CI, 9CI) (CA INDEX NAME)



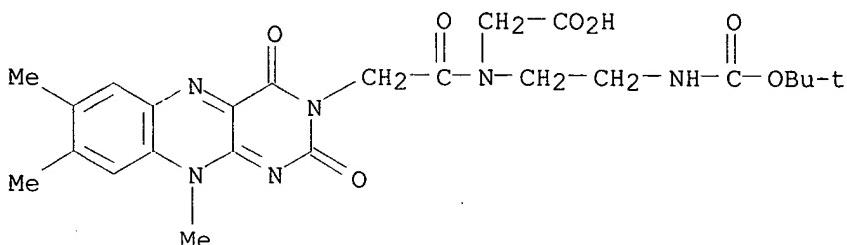
RN 340259-04-3 CAPPLUS

CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



RN 340259-05-4 CAPPLUS

CN Glycine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-N-[2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 4 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:691862 CAPLUS

DOCUMENT NUMBER: 132:10368

TITLE: On the photoinactivation of alcohol oxidase from alkane-grown *Candida tropicalis*

AUTHOR(S): Dickinson, Francis M.

CORPORATE SOURCE: Department of Biological Sciences, University of Hull, Hull, HU6 7RX, UK

SOURCE: J. Photochem. Photobiol., B (1999), 50(2-3), 144-148
CODEN: JPPBEG; ISSN: 1011-1344

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The process of photoinactivation of alc. oxidase is insensitive to oxygen and to temp. in the range 0-25.degree.C. The process is, however, wavelength dependent. Irradn. and inactivation do not cause any significant change to the visible absorption spectrum. Reaction of the enzyme with sodium sulfite or photoredn. in the presence of EDTA and either 5'-deazaflavin or lumiflavin 3-acetate under anaerobic conditions causes extensive bleaching of the visible spectrum of the enzyme and also protects it from photoinactivation. The presence of substrate under anaerobic conditions also provides very effective protection, but in this case there is no detectable change in the visible spectrum of the enzyme assocd. with the increase in stability to light.

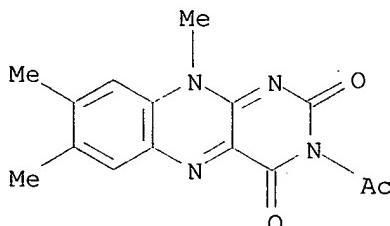
IT 60823-53-2

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(protection of alc. oxidase from photoinactivation)

RN 60823-53-2 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-acetyl-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 5 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:361752 CAPLUS

DOCUMENT NUMBER: 129:117429

TITLE: Synthesis, DNA-binding properties and cytotoxic activity of flavin-oligopyrrolecarboxamide and flavin-oligoimidazolecarboxamide conjugates

AUTHOR(S): Herfeld, Philippe; Helissey, Philippe; Nafziger, Joelle; Giorgi-Renault, Sylviane

CORPORATE SOURCE: Lab. Chimie Therapeutique, Univ. Rene Descartes, Paris, 75270, Fr.

SOURCE: Anti-Cancer Drug Design (1998), 13(4), 337-359

CODEN: ACDDEA; ISSN: 0266-9536

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The aim of this study was to develop novel series of photosensitizer-DNA minor groove binder hybrids composed of a flavin (isoalloxazine) chromophore linked to a moiety related to netropsin or distamycin. Three series (Fla-Pyr, Fla-Gly-Pyr and Fla-Gly-Im) were synthesized which differ by the no. and the nature of the heterocyclic nuclei in the oligopeptide units, the nature of the linker and its anchoring position on the flavin. In terms of DNA binding and DNA specificity, satisfactory data are obtained in the Fla-Pyr and Fla-Gly-Pyr series; in terms of photo-induced cytotoxicity, the results are disappointing. The present study allows us to draw the following structure-activity relationships: (i) substitution of the flavin nucleus in either the N3 or the N10 position does not affect the activity; (ii) tris-pyrrolic hybrids are more efficient than bis- and tetra-pyrrolic analogs; (iii) the presence of a glycine in the linking chain does not suppress the DNA binding properties or the cytotoxic activities of the hybrids; and (i.v.) the replacement of the pyrrole nuclei by imidazoles has a drastic effect since it results in the loss of DNA affinity and cytotoxicity.

IT 144446-13-9 144446-14-0

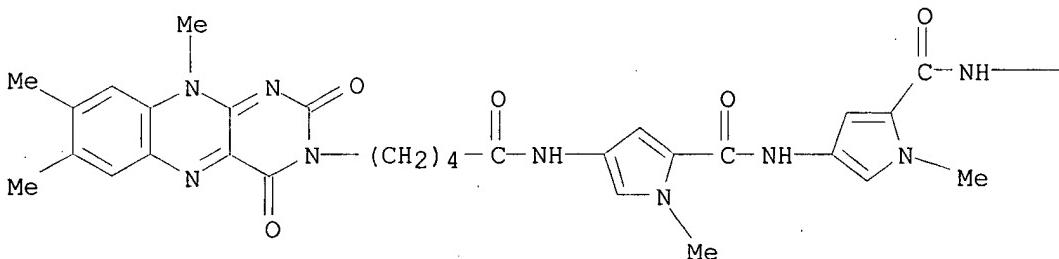
RL: BPR (Biological process); PRP (Properties); BIOL (Biological study);
PROC (Process)

(prepn. and DNA-binding properties and cytotoxic activity of
flavin-oligopyrrolecarboxamide and flavin-oligoimidazolecarboxamide
conjugates)

RN 144446-13-9 CAPLUS

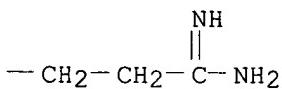
CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



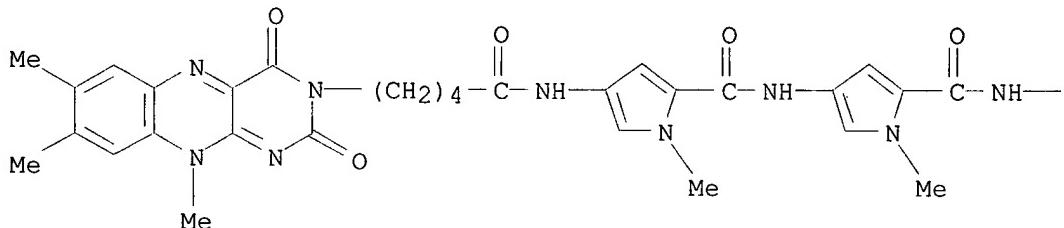
HCl

PAGE 1-B



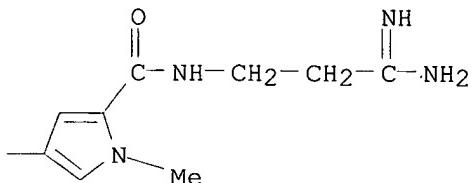
RN 144446-14-0 CAPLUS
CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[5-[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)

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• HCl

PAGE 1-B



L37 ANSWER 6 OF 72 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:444645 CAPLUS
DOCUMENT NUMBER: 125:135669
TITLE: Binding of Net-Fla, a netropsin-flavin hybrid molecule, to DNA: Molecular mechanics and dynamics studies in vacuo and in water solution
AUTHOR(S): Ketterle, Christophe; Gabarro-Arpa, Jacques; Bouziane, Mohammed; Auclair, Christian; Helissey, Philippe; Giorgi-Renault, Sylviane; Le Bret, Marc
CORPORATE SOURCE: Lab. Physicochim., Institut Gustave Roussy, Villejuif, 94805, Fr.
SOURCE: J. Biomol. Struct. Dyn. (1996), 13(6), 963-977
CODEN: JBSDD6; ISSN: 0739-1102
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have studied the binding of the hybrid netropsin-flavin (Net-Fla) mol. onto four sequences contg. four A.T base pairs. Mol. mechanics

minimizations in vacuo show numerous minimal conformations sep'd. by one base pair. 400 Ps mol. dynamics simulations in vacuo have been performed using the lowest min. as the starting conformations. During these simulations, the flavin moiety of the drug makes two hydrogen bonds with an amino group of a neighboring guanine. A 200 ps mol. dynamics simulation in explicit water soln. suggests that the binding of Net-Fla upon the DNA substrate is enhanced by water bridges. A water mol. bridging the amidinium of Net-Fla to the N3 atom of an adenine seems to be stuck in the drug-DNA complex during the whole simulation. The fluctuations of the DNA helical parameters and of the torsion angles of the sugar-phosphate backbone are very similar in the simulations in vacuo and in water. The time auto-correlation functions for the DNA helical parameters decrease rapidly in the picosecond range in vacuo. The same functions computed from the water soln. mol. dynamics simulations seem to have two modes: the rapid mode is similar to the behavior in vacuo, and is followed by a slower mode in the 10 ps range.

IT 179598-32-4D, Net-Fla, complex with DNA

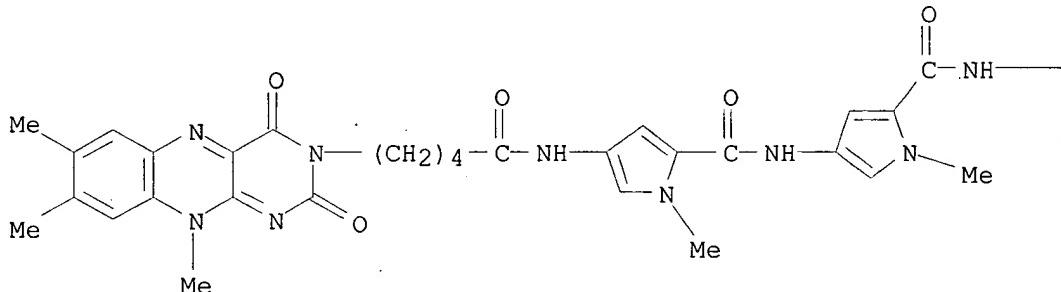
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(mol. mechanics and dynamics simulations of binding of netropsin-flavin hybrid mol. Net-Fla to A-T-rich DNA in vacuo and in water soln.)

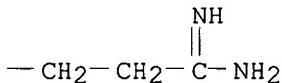
RN 179598-32-4 CAPLUS

CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)

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PAGE 1-B



L37 ANSWER 7 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:861545 CAPLUS

DOCUMENT NUMBER: 124:3227

TITLE: Sequence-directed single strand cleavage of DNA by a netropsin-flavin hybrid molecule

AUTHOR(S): Bouziane, Mohammed; Ketterle, Christophe; Helissey, Philippe; Herfeld, Philippe; Le Bret, Marc; Giorgi-Renault, Sylviane; Auclair, Christian

CORPORATE SOURCE: Laboratoire de Physicochimie et Pharmacologie des Macromolecules Biologiques, Institut Gustave Roussy, Villejuif, 94805, Fr.

SOURCE: Biochemistry (1995), 34(43), 14051-8

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB In an attempt to obtain sequence-specific DNA-cleaving mol., a series of hybrid minor groove binders were synthesized composed of a photoactiveable isoalloxazine (flavin) chromophore linked through a polymethylenic chain to a bis-pyrrolecarboxamide moiety related to netropsin. Like netropsin, the hybrid derivs. preferentially bind to A+T-rich sequences. Activation of the flavin chromophore by visible light results in the appearance of single strand breaks in the vicinity of the DNA binding site. The cleavage affinity properties of one of these compds. referred to as netropsin-flavin (Net-Fla) and considered as representative of the series was further investigated. Net-Fla cleaves only one strand at a specific locus downstream of 5'-AAAT-3', upstream of 5'-TAAA-3' and on either side of a 5'-AAAA-3' sequence. Net-Fla cleaves both strands downstream to 5'-AATT-3'. This makes the properties of Net-Fla similar to that of a restriction endonuclease and provides addnl. insight into establishing the rules for the readout of B-DNA helix by non-nucleotidic compds. Mol. modeling showed that Net-Fla binds to an asym. site in one orientation. The values of the energetic min. lie in the same order as expected from the cleavage patterns, which suggests that the oriented cleavage is a consequence of a sequence-oriented binding of Net-Fla in the DNA minor groove.

IT 144446-13-9

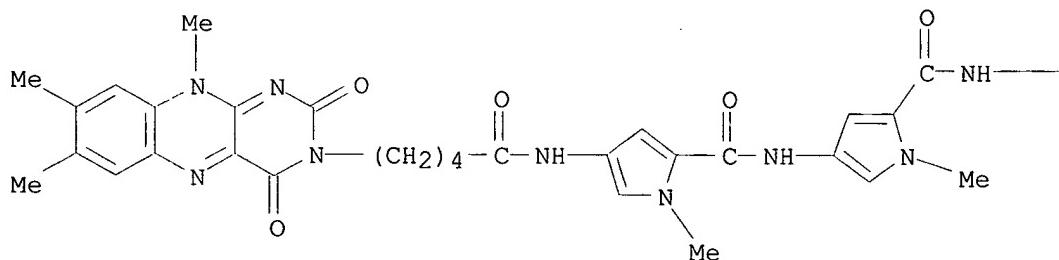
RL: CAT (Catalyst use); USES (Uses)

(sequence-directed single strand cleavage of DNA by a netropsin-flavin hybrid mol.)

RN 144446-13-9 CAPLUS

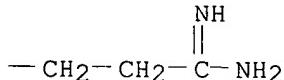
CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



● HCl

PAGE 1-B



L37 ANSWER 8 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1995:538956 CAPLUS
 DOCUMENT NUMBER: 123:29795

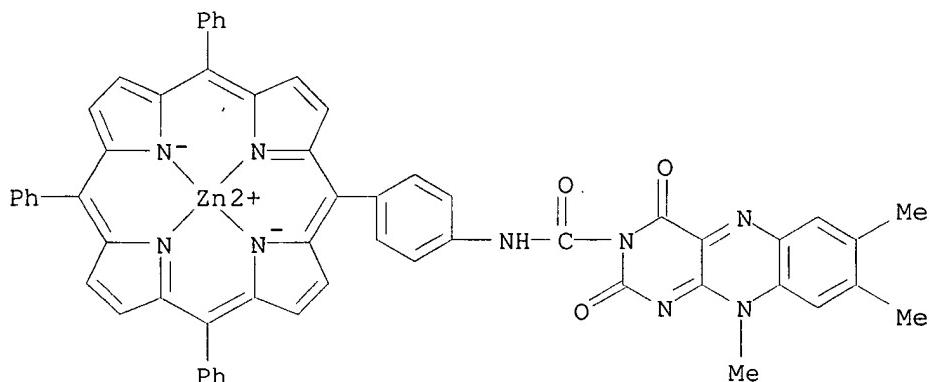
TITLE: Molecular Architecture and Environmental Effects in Intramolecular Electron Transfer. An Electron Paramagnetic Resonance Study
 AUTHOR(S): Hasharoni, Kobi; Levanon, Haim; Gaetschmann, Joerg; Schubert, Heike; Kurreck, Harry; Moebius, Klaus
 CORPORATE SOURCE: Department of Physical Chemistry, Hebrew University of Jerusalem, Jerusalem, 91904, Israel
 SOURCE: J. Phys. Chem. (1995), 99(19), 7514-21
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Intramol. electron transfer (ET) in three photosynthetic model systems, oriented in liq. crystals (LCs), was monitored by continuous wave time-resolved ESR (CW-TREPR) spectroscopy: (1) zinc porphyrin (ZnTPP) linked via an amide spacer to a lumiflavin (PaF); (2) ZnTPP linked to a benzoquinone via a Ph spacer in the para (p-PpQ); and (3) in the meta (m-PpQ) positions. The anisotropic liq. cryst. environment makes the ET products detectable over a wide range of temps., i.e., 210 $\text{K} \leq T \leq 330 \text{ K}$. Under such exptl. conditions the ET rates are reduced quite dramatically into the solvent controlled adiabatic regime. The spectral line shape differences reflect the effect of the mol. architecture, namely, the relative orientation of the donor-acceptor as well as the spacer moiety. These differences in mol. structures are manifested by the TREPR spectra through the magnitude of the spin-spin coupling (J) and the dipolar interaction (D), thus leading to different electron spin polarization mechanisms.

IT 164120-87-0

RL: BPR (Biological process); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
 (intramol. electron transfer in covalently linked porphyrin-spacer-quinone model photosystems)

RN 164120-87-0 CAPLUS

CN Zinc, [4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-N-[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl]benzo[g]pteridine-3(2H)-carboxamidato(2-)-N21,N22,N23,N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



L37 ANSWER 9 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1995:466170 CAPLUS
 DOCUMENT NUMBER: 123:97552
 TITLE: Attenuation of Intramolecular Electron Transfer Rates in Liquid Crystals
 AUTHOR(S): Hasharoni, Kobi; Levanon, Haim
 CORPORATE SOURCE: Department of Physical Chemistry, The Hebrew University, Jerusalem, 91904, Israel
 SOURCE: J. Phys. Chem. (1995), 99(14), 4875-8

CODEN: JPCHAX; ISSN: 0022-3654

DOCUMENT TYPE:

Journal

LANGUAGE:

English

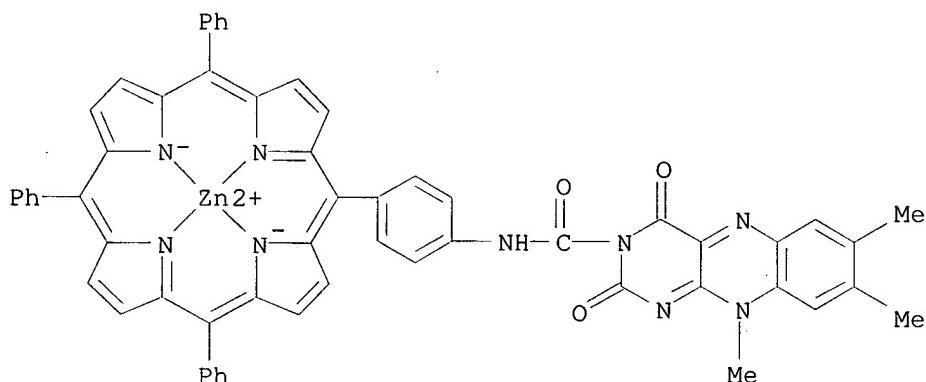
AB The anisotropic properties of liq. crystals (LC) are the key factor in reducing photoinduced intramol. electron transfer (IET) rates in donor-spacer-acceptor systems. A rate redn. by 3-4 orders of magnitude in LCs, as compared to normal isotropic liqs., enables to apply submicrosecond EPR spectroscopy to these reactions. We attribute this remarkable effect to the existence of a potential barrier, known as the nematic potential, which characterizes the anisotropic nature of the nematic LC. This nematic potential slows the rotational correlation time of the liq. cryst. solvent mol. dipoles. Since IET is coupled to the solvent motion, slowing the rotational correlation time reduces the IET rate. Moreover, in all cases examd., the solvent (LC) dynamics control the IET rate over the entire nematic phase, thus suggesting that the reaction dynamics is brought into the solvent-controlled adiabatic limit.

IT 164120-87-0

RL: PEP (Physical, engineering or chemical process); PROC (Process)
(attenuation of intramol. electron transfer rates in liq. crystals)

RN 164120-87-0 CAPLUS

CN Zinc, [4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-N-[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl]benzo[g]pteridine-3(2H)-carboxamidato(2-)-N21,N22,N23,N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



L37 ANSWER 10 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:95688 CAPLUS

DOCUMENT NUMBER: 120:95688

TITLE: Poly(pyrrolecarboxamides) linked to photoactivatable chromophore isoalloxazine. Synthesis, selective binding, and DNA cleaving properties

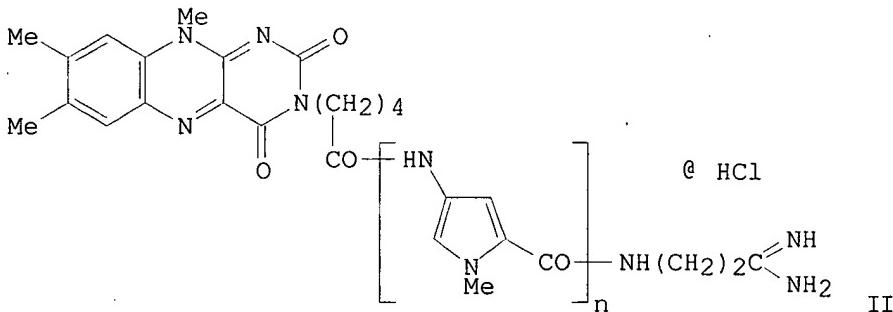
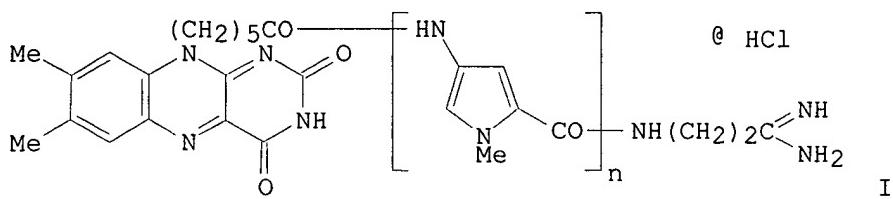
AUTHOR(S): Herfeld, Philippe; Helissey, Philippe; Giorgi-Renault, Sylviane; Goulaouic, Helene; Pager, Jeanne; Auclair, Christian

CORPORATE SOURCE: Lab. Chim. Ther., Fac. Sci. Pharm. Biol., Paris, 75270, Fr.

SOURCE: Bioconjugate Chem. (1994), 5(1), 67-76
CODEN: BCCHE8; ISSN: 1043-1802

DOCUMENT TYPE: Journal
LANGUAGE: English

GI



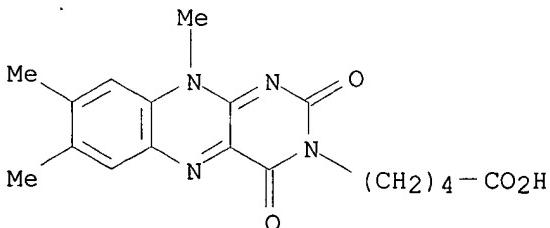
AB In an attempt to obtain DNA sequence-specific cleaving mols., the authors prep'd. 2 types of hybrid groove binders composed of an isoalloxazine (flavin) chromophore linked through a polymethylenic chain to either a bis- or a tris(pyrrolecarboxamide) moiety related to netropsin and distamycin, resp. In both types of mols., the polymethylenic chain was linked to the alloxazine ring either in the N-10 position (I, e.g., n = 2) or in the N-3 position (II, e.g., n = 2). As netropsin and distamycin, the hybrid derivs. preferentially bound to A + T-rich sequences and recognize sequences such as 5'-ATTT. Upon visible light irradn. the flavin moiety undergoes a redox cycling process generating superoxide anion and hydroxyl radical. Generation of oxy radicals appears to be more efficient with the hybrids in which the polymethylenic chain is linked at the N-10 position. The generation of oxy radicals results in the occurrence of single strand break in supercoiled DNA. Breaks preferentially occur in the vicinity of A + T-rich sequences. The advantage of flavin relative to other oxy radicals generating compds. such as ferrous-EDTA is that it does not require chem. redn. but can be reduced either by visible light or by cellular enzymes, both conditions being compatible with pharmacol. constraints.

IT 144446-18-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and amidation of, by aminopyrrolecarboxamide derivs.)

RN 144446-18-4 CAPLUS

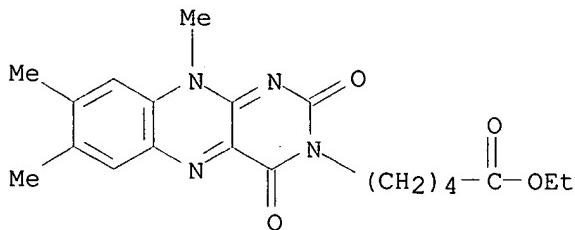
CN Benzo[g]pteridine-3(2H)-pentanoic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



IT 144446-17-3P

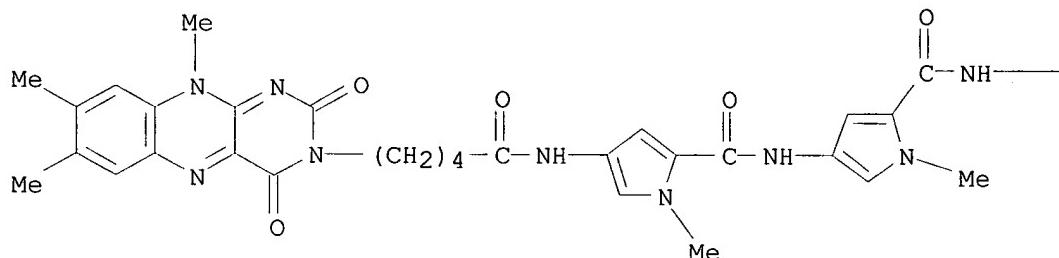
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

RN 144446-17-3 CAPLUS
 CN Benzo[g]pteridine-3(2H)-pentanoic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



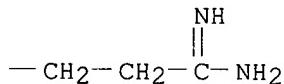
IT 144446-13-9P 144446-14-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and selective binding and DNA cleaving properties of)
 RN 144446-13-9 CAPLUS
 CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



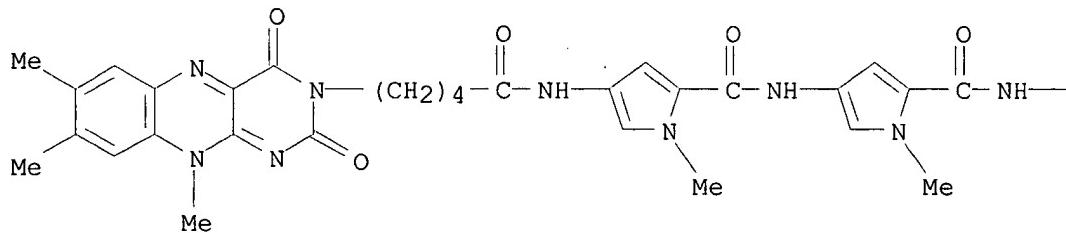
● HCl

PAGE 1-B



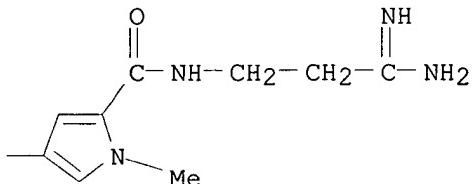
RN 144446-14-0 CAPLUS
 CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[[5-[[[3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



● HCl

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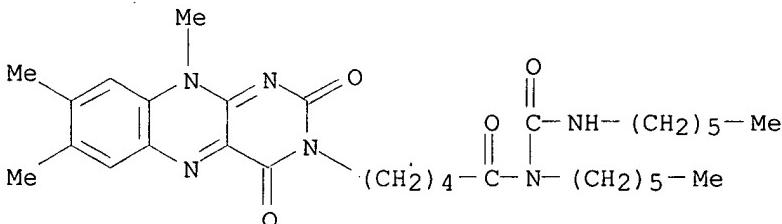


IT 152721-23-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 152721-23-8 CAPLUS

CN Benzo[g]pteridine-3(2H)-pentanamide, N-hexyl-N-[(hexylamino)carbonyl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



L37 ANSWER 11 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:649764 CAPLUS

DOCUMENT NUMBER: 119:249764

TITLE: The mechanism of adduct formation between reduced
flavins and arene epoxides

AUTHOR(S): Lee, Yong T.; Fisher, Jed F.

CORPORATE SOURCE: Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455,
USA

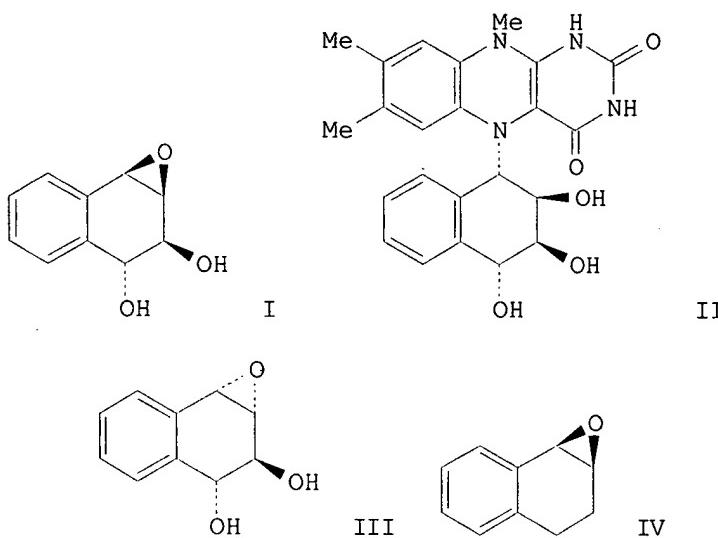
SOURCE: J. Org. Chem. (1993), 58(14), 3712-21

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The mechanism of nucleophilic epoxide opening by reduced flavins, a potentially relevant transformation to the carcinogenesis of polycyclic arom. hydrocarbons, was investigated. In the spontaneous epoxide hydrolysis pH region, the reaction pathway between the epoxide and the dihydroflavin is bimol. epoxide opening. Chromatog. anal. of the reaction of (.+.)-1a,2,3,7b-tetrahydro-(1a.alpha.,2.alpha.,3.beta.,7b.alpha.)-naphth[1,2-b]oxirene-2,3-diol (I) with 5,10-dihydro-7,8,10-trimethylbenzo[g]pteridine-2,4(1H,3H)-dione (LFH₂, dihydrolumiflavin) in 9/1 (vol./vol.) aq. pH 7.86 Tris buffer-dioxane yielded the flavin N(5) adduct II as the only major product. Under the same conditions, arene epoxide III gave the N(5) adduct, N(3) adducts, and an unknown adduct possibly the C(4a) adduct, each in similar yields. The tetrahydronaphthalene oxide IV gave the N(5) adduct and the C(4a) adduct in approx. a 2/1 ratio. The C(4a) adduct was not stable, however, and was transformed to a secondary adduct. A comparison of the absorption spectra indicated that the outcome of I and IV with FMNH₂ was similar to that for LFH₂. The reaction of III with FMNH₂ gave an adduct, assigned to that from C(4a) adduct, in addn. to the N(5) and N(3) adducts. While the reactions of I (pH 5.1) and III (pH 4.3) with LFH₂ under acidic conditions gave only the N(5) adducts, that of IV at pH 6.6 gave the same adducts as obsd. at pH 7.86. Most of these adducts have been isolated. All but one of the adducts exhibited trans stereochem. with respect to epoxide opening. Rate consts. for these reactions were detd. by chromatog. monitoring of the epoxide disappearance and for these epoxides in the spontaneous region (pH approx. 7.5) are in the range of 0.1-0.5 M⁻¹s⁻¹. The magnitude of these rate consts. indicates that the rate const. for nucleophilic, bimol. attack by the dihydrflavin on these epoxides is comparable to that of the thiolate anion. The behavior of the epoxides with the dihydroflavins provides one of the few quant. ests. of the nucleophilic capacity of the dihydroflavin and confirms the perception of the dihydroflavin as an exceptionally reactive nucleophile.

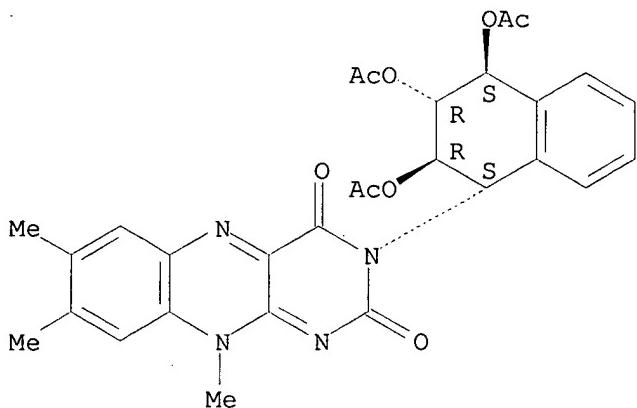
IT 149520-22-9P 149562-16-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 149520-22-9 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-[2,3,4-tris(acetoxy)-1,2,3,4-tetrahydro-1-naphthalenyl]-, (1.alpha.,2.beta.,3.alpha.,4.beta.)- (9CI) (CA INDEX NAME)

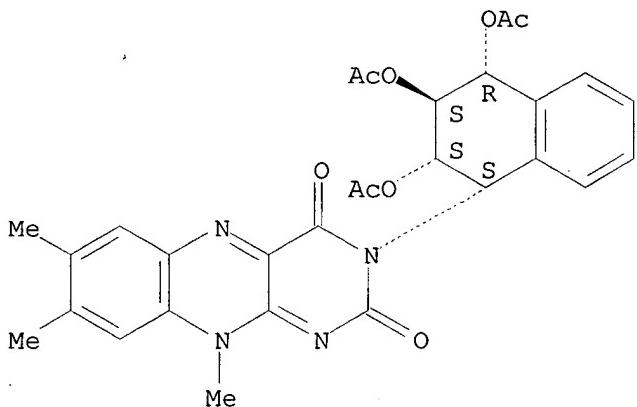
Relative stereochemistry.



RN 149562-16-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-[2,3,4-tris(acetoxy)-1,2,3,4-tetrahydro-1-naphthalenyl]-, (1.alpha.,2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L37 ANSWER 12 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:549291 CAPLUS

DOCUMENT NUMBER: 119:149291

TITLE: A fluorescence study of lumichrome phototautomerism in dodecylammonium propionate reversed micelles

AUTHOR(S): Tyrakowska, B.; Bastiaens, P. I. H.; Koziolowa, A.; Visser, A. J. W. G.

CORPORATE SOURCE: Institute of Commodity Science, Poznan University of Economics, Poznan, Pol.

SOURCE: J. Photochem. Photobiol., A (1993), 72(3), 235-41
CODEN: JPPCEJ; ISSN: 1010-6030

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Spectral and time-resolved polarized fluorescence expts. were carried out on N(3)-undecyl-lumichrome and N(3)-undecyl-lumiflavin encapsulated in reversed micelles of dodecylammonium propionate in cyclohexane. The compds. were equipped with a long chain to anchor them to the interphase boundary between the water droplet and the org. phase. The spectral expts. revealed that the amphiphilic compds. were located at the interphase. The observation that the propionate counter-ion of the

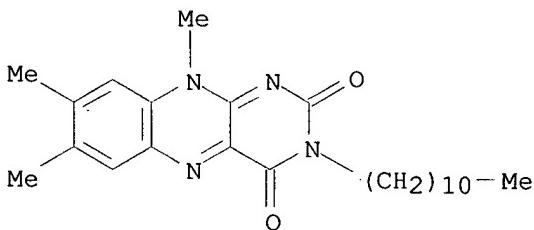
micellar ammonium head group enables phototautomerism to yield isoalloxazinic fluorescence provided evidence for the close contact of lumichrome with propionate. Dynamic information was obtained from a two-dimensional max. entropy method of anal. of the time-resolved fluorescence data of flavin and phototautomeric lumichrome. On the basis of these results it was clear that the fluorophores were distributed differently within the micellar boundary region.

IT 73057-72-4

RL: PRP (Properties)

(phototautomerism of, in reversed micelles, fluorescence study of)

RN 73057-72-4 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-undecyl- (9CI)
(CA INDEX NAME)

L37 ANSWER 13 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:633715 CAPLUS

DOCUMENT NUMBER: 117:233715

TITLE: Preparation of (isoalloxazinoalkyl)netropsins and -distamycins as cytotoxic agents

INVENTOR(S): Auclair, Christian; Giorgi-Renault, Sylviane; Helissey, Philippe; Paoletti, Claude

PATENT ASSIGNEE(S): Centre National de la Recherche Scientifique, Fr.; Institut Gustave Roussy

SOURCE: Fr. Demande, 33 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

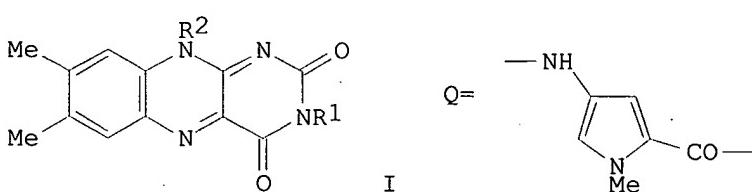
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2666088	A1	19920228	FR 1990-10594	19900823
FR 2666088	B1	19921211		

OTHER SOURCE(S): MARPAT 117:233715

GI



AB Title compds. [I; R1 = (CH2)mCOZnNHCH2CH2C(:NH)NH2.HX and R2 = Me; R1 = H and R2 = (CH2)mCOZnNHCH2CH2C(:NH)NH.HX; X = pharmaceutically acceptable anion; Z = iminopyrrolylenecarbonyl group Q; m = 1-6; n = 1-4] were prep'd.

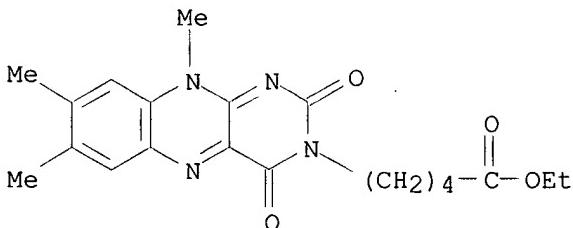
Thus, I [R1 = (CH₂)₄CO₂H, R2 = Me] (prepn. given) was condensed with HZ₂NHCH₂CH₂C(:NH)NH₂.HCl (Z = Q) to give I [R1 = (CH₂)₄CO₂NHCH₂CH₂C(:NH)NH₂.HCl, R2 = Me, Z = Q] which gave apprx.3 times as much cleavage of plasmid pBR322 as that given by riboflavin after 10 min irradn.

IT 144446-17-3P 144446-18-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of cytotoxic agent)

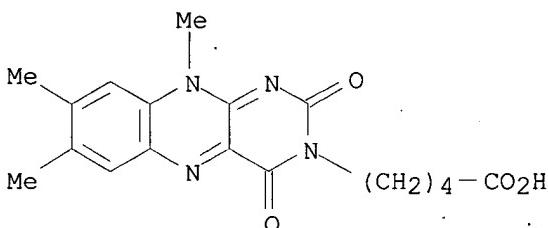
RN 144446-17-3 CAPLUS

CN Benzo[g]pteridine-3(2H)-pentanoic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 144446-18-4 CAPLUS

CN Benzo[g]pteridine-3(2H)-pentanoic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



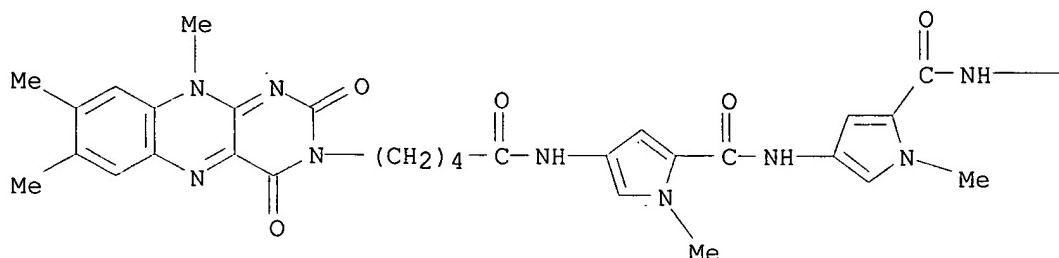
IT 144446-13-9P 144446-14-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cytotoxic agent)

RN 144446-13-9 CAPLUS

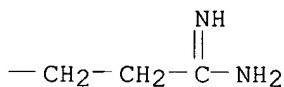
CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



● HCl

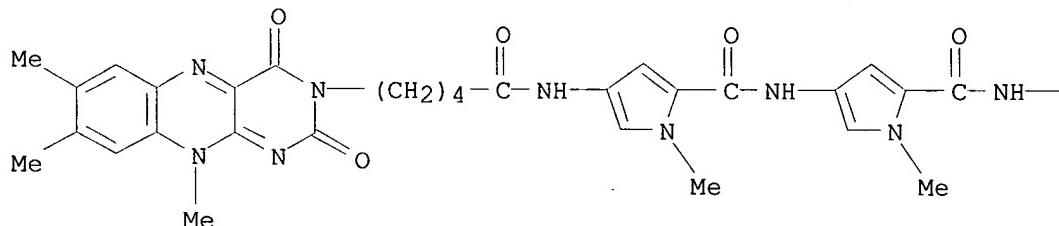
PAGE 1-B



RN 144446-14-0 CAPLUS

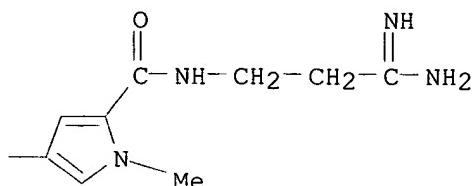
CN Benzo[g]pteridine-3(2H)-pentanamide, N-[5-[[[5-[[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



● HCl

PAGE 1-B



L37 ANSWER 14 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1992:129748 CAPLUS
 DOCUMENT NUMBER: 116:129748
 TITLE: Flavin-containing polyanions; synthesis, activity, and immobilization in polyelectrolyte complexes
 AUTHOR(S): Schoo, Herman F. M.; Challa, Ger
 CORPORATE SOURCE: Lab. Polym. Chem., Univ. Groningen, Groningen, 9747 AG, Neth.
 SOURCE: Macromolecules (1992), 25(6), 1633-8
 CODEN: MAMOBX; ISSN: 0024-9297
 DOCUMENT TYPE: Journal
 LANGUAGE: English

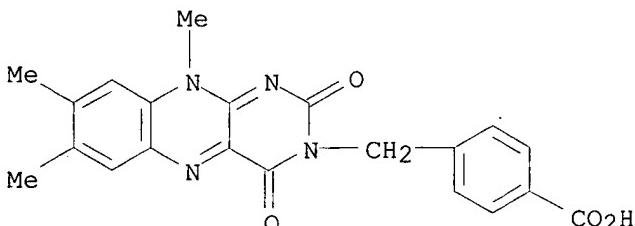
AB Linear polymers contg. both flavin units and COOH groups were prep'd. by copolymer. of the appropriate styrene derivs. The catalytic activity of the resulting polyanions in aq. media was detd. for the aerobic oxidn. of 1-benzyl-1,4-dihydronicotinamide. A 69-fold (max.) increase of the activity of the flavin moieties was found after binding to the polyanions as compared to a low molar mass analog, which may be attributed to a higher polarity of the microenvironment of the catalyst and to H bonding of the flavin units to the COOH groups. The activity of the polyanions was dependent on the pH of the medium, with an optimum at pH apprxeq. 8. Complexation of the polyanions with polycations contg. pendent quaternary ammonium groups led to a small decrease in activity, the effect being larger with a higher charge d. of the polycation. The resulting polyelectrolyte complex gel particles were quite stable and could be used in a continuous reaction for many days without loss of activity. Finally, homopolymer. of the flavin-contg. monomer resulted in the 1st flavin homopolymer.

IT 138835-38-8

RL: CAT (Catalyst use); USES (Uses)
 (catalysts, for aerobic oxidn. of benzylidihydronicotinamide, as model for flavin-contg. polyanions)

RN 138835-38-8 CAPLUS

CN Benzoic acid, 4-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)methyl]- (9CI) (CA INDEX NAME)



IT 138835-39-9DP, hydrolyzed, compds. with chloromethylated polystyrene compd. with triethylamine

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (catalysts, prepn. and activity of, for aerobic oxidn. of benzylidihydronicotinamide)

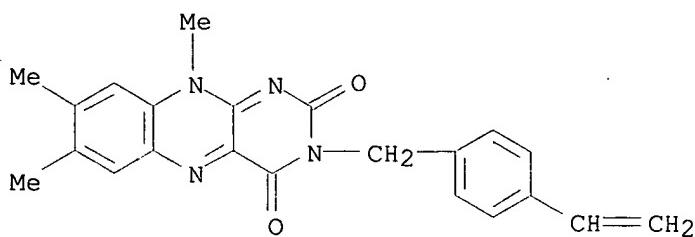
RN 138835-39-9 CAPLUS

CN Benzoic acid, 4-ethenyl-, 1,1-dimethylethyl ester, polymer with 3-[(4-ethenylphenyl)methyl]-7,8,10-trimethylbenzo[g]pteridine-2,4(3H,10H)-dione (9CI) (CA INDEX NAME)

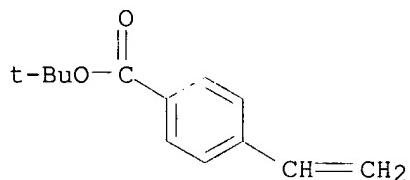
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CRN 136951-08-1

CMF C22 H20 N4 O2



CM 2

CRN 84740-98-7
CMF C13 H16 O2

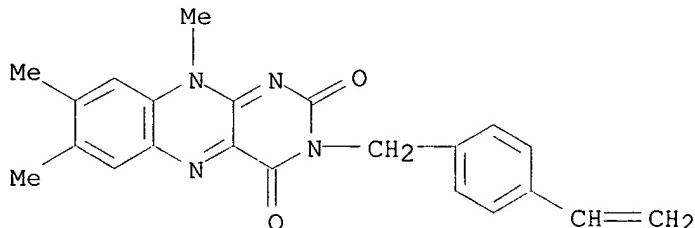
IT 138835-40-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and characterization of)

RN 138835-40-2 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-[(4-ethenylphenyl)methyl]-7,8,10-trimethyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 136951-08-1
CMF C22 H20 N4 O2

IT 138835-39-9P

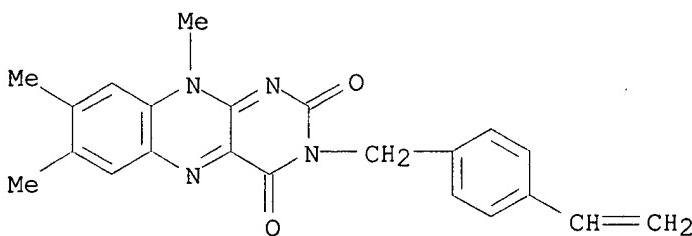
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

RN 138835-39-9 CAPLUS

CN Benzoic acid, 4-ethenyl-, 1,1-dimethylethyl ester, polymer with
3-[(4-ethenylphenyl)methyl]-7,8,10-trimethylbenzo[g]pteridine-2,4(3H,10H)-
dione (9CI) (CA INDEX NAME)

CM 1

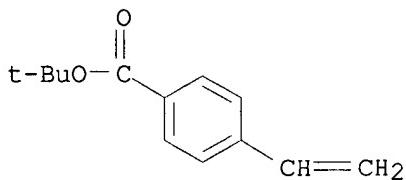
CRN 136951-08-1
CMF C22 H20 N4 O2



CM 2

CRN 84740-98-7

CMF C13 H16 O2

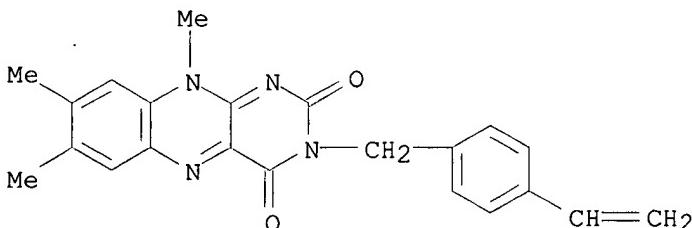


IT 136951-08-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and polymn. of, with tert-Bu vinylbenzoate)

RN 136951-08-1 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-[(4-ethenylphenyl)methyl]-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 15 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:427901 CAPLUS

DOCUMENT NUMBER: 119:27901

TITLE: Synthesis of flavins bearing a sulfur functional group
and their catalytic activities for reduction of
disulfides

AUTHOR(S): Nagata, Toshiyuki; Fujimori, Ken; Oae, Shigeru

CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan

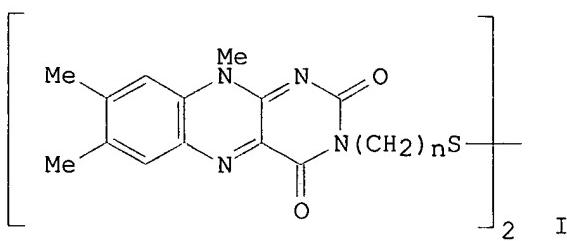
SOURCE: Heteroat. Chem. (1992), 3(5-6), 617-24

CODEN: HETCE8; ISSN: 1042-7163

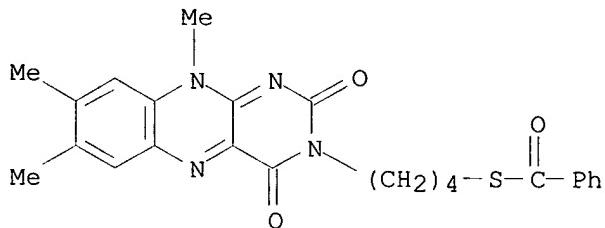
DOCUMENT TYPE: Journal

LANGUAGE: English

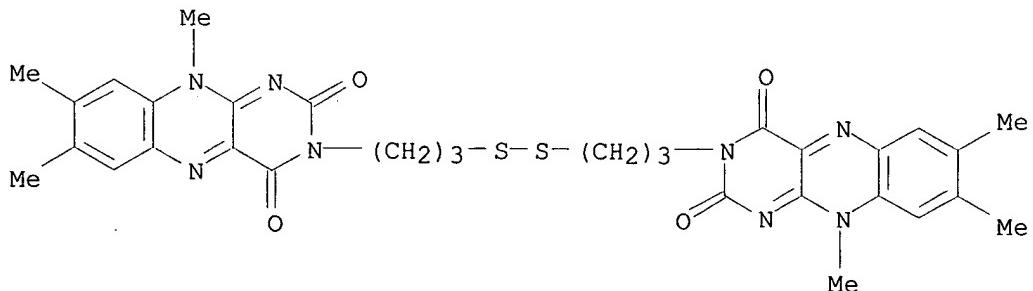
GI



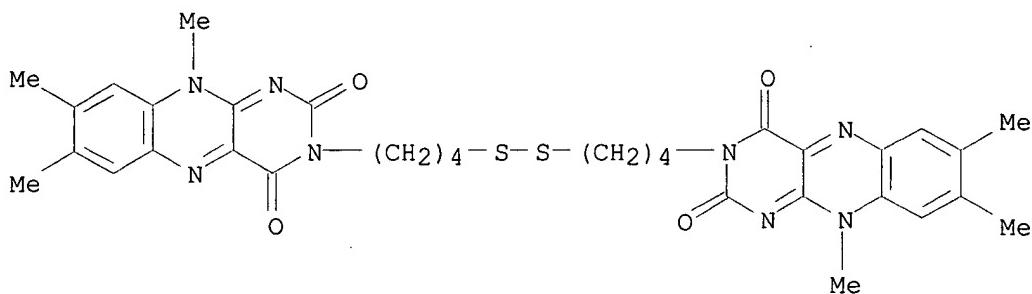
- AB Bis-flavins I ($n = 3-6$), each of which bears a disulfide linkage in the mol., have been synthesized as model compds. for dihydronicotinamide dependent disulfide reductase. These flavins were found to be much better catalysts to promote the redn. of dibenzyl disulfide to α -toluenethiol than 3-methylllumiflavin.
- IT **147874-83-7P**, 3-(4-Benzoylthiobutyl)lumiflavin
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and ammonolysis and oxidn. of, disulfide from)
- RN 147874-83-7 CAPLUS
- CN Benzenecarbothioic acid, S-[4-(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)butyl] ester (9CI) (CA INDEX NAME)



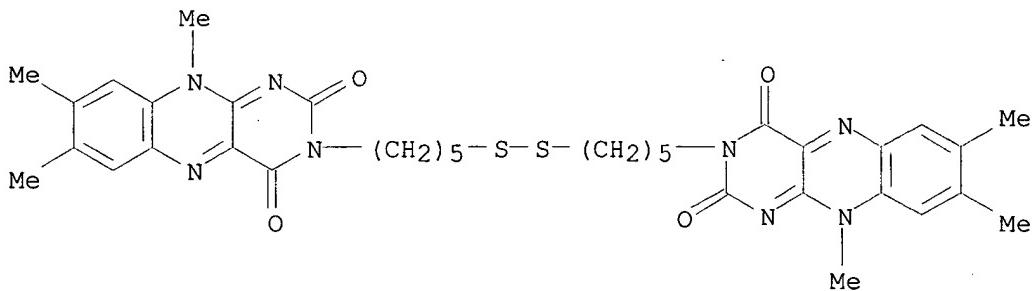
- IT **147874-78-0P 147874-79-1P 147874-80-4P**
147874-81-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and catalytic activity of, in the redn. of dibenzyl disulfide)
- RN 147874-78-0 CAPLUS
- CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3,3'-(dithiodi-3,1-propanediyl)bis[7,8,10-trimethyl- (9CI) (CA INDEX NAME)



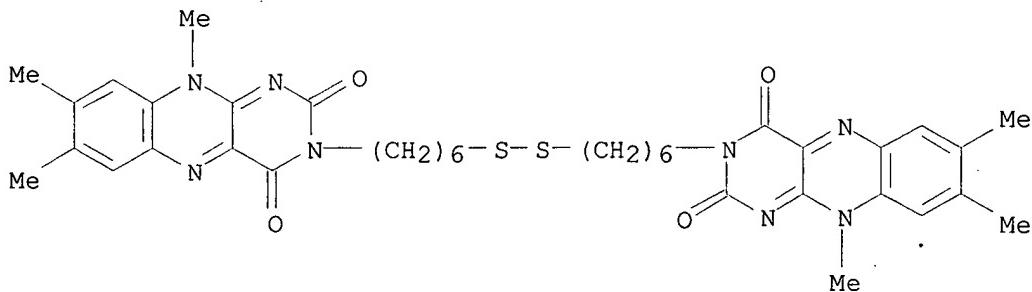
- RN 147874-79-1 CAPLUS
- CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3,3'-(dithiodi-4,1-butanediyl)bis[7,8,10-trimethyl- (9CI) (CA INDEX NAME)



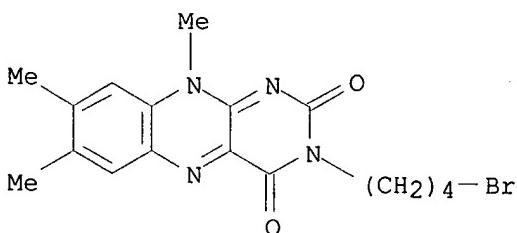
RN 147874-80-4 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3,3'-(dithiodi-5,1-pentanediyi)bis[7,8,10-trimethyl- (9CI) (CA INDEX NAME)



RN 147874-81-5 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3,3'-(dithiodi-6,1-hexanediyi)bis[7,8,10-trimethyl- (9CI) (CA INDEX NAME)



IT 147874-82-6P, 3-(4-Bromobutyl)lumiflavin
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and substitution reaction of, with thiobenzoic acid)
 RN 147874-82-6 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-(4-bromobutyl)-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 16 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:465742 CAPLUS

DOCUMENT NUMBER: 117:65742

TITLE: Electrochemically prepared polyelectrolyte complex of polypyrrole and flavin-containing polyanion. Use as a biosensor

AUTHOR(S): Schoo, H. F. M.; Challa, G.

CORPORATE SOURCE: Lab. Polym. Chem., Univ. Groningen, Groningen, 9747 AG, Neth.

SOURCE: ACS Symp. Ser. (1992), 487(Biosens. Chem. Sens.), 164-74

CODEN: ACSMC8; ISSN: 0097-6156

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Pyrrole was polymd. electrochem. in an aq. medium on a platinum electrode in the presence of a polyanion, contg. covalently bound flavin units. Depending on the applied potential the polypyrrole-films thus formed were powd. and non-adherent ($V < 700$ mV), smooth and adherent (700 mV $< V < 1000$ mV) or brittle and uneven ($V > 1000$ mV). Besides the applied potential, medium pH and added low molar mass salt influenced the morphol. and compn. of the PPy-layer. The flavin-contg. polyanion was incorporated in the film as a dopant. Depending on the medium pH and amt. of low molar mass salt added, the film formed by this method contained various amts. of polymer-bound flavin. Cyclic voltammograms confirmed the presence of electrochem. active flavin in the layer. The oxidn. of 1-benzyl-1,4-dihydronicotinamide (BNAH) was used as a model reaction to test the catalytic activity of the immobilized flavin. The modified electrode showed fast current response on addn. of BNAH, not only at an applied potential of 0.9 V (oxidn. of H₂O₂) but also in the absence of oxygen at 0.3 V. This might indicate that a direct transfer of electrons takes place between the flavin units and the (PPy-)electrode. Cycling of the PPy-film through its reduced and oxidized state does not lead to any loss of the flavin contg. polyanion. In the case of low molar mass flavin-contg. dopants most of the flavin is released from the film upon redn. of the PPy.

IT 136951-09-2DP, complexes with polypyrrole

RL: PREP (Preparation)

(prepn. and application in electrode)

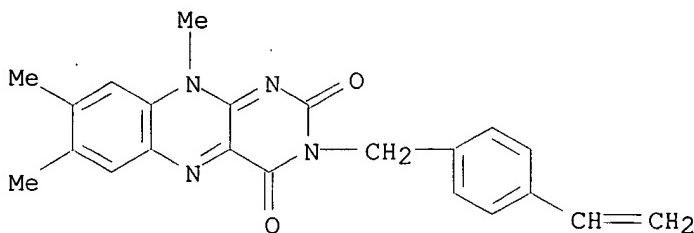
RN 136951-09-2 CAPLUS

CN Benzoic acid, 4-ethenyl-, polymer with 3-[(4-ethenylphenyl)methyl]-7,8,10-trimethylbenzo[g]pteridine-2,4(3H,10H)-dione (9CI) (CA INDEX NAME)

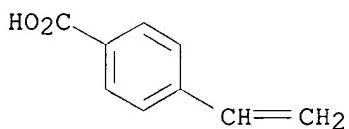
CM 1

CRN 136951-08-1

CMF C22 H₂O N4 O2



CM 2

CRN 1075-49-6
CMF C9 H8 O2

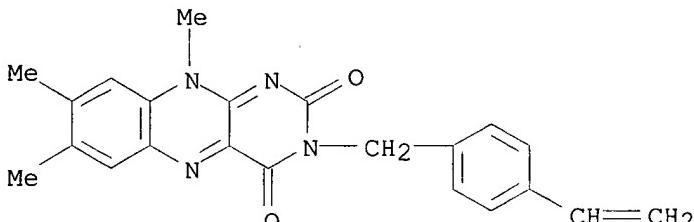
IT 136951-09-2

RL: RCT (Reactant)
(reaction of, with polymd. pyrrole)

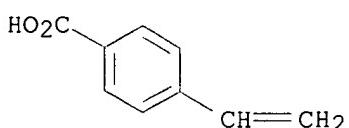
RN 136951-09-2 CAPLUS

CN Benzoic acid, 4-ethenyl-, polymer with 3-[(4-ethenylphenyl)methyl]-7,8,10-trimethylbenzo[g]pteridine-2,4(3H,10H)-dione (9CI) (CA INDEX NAME)

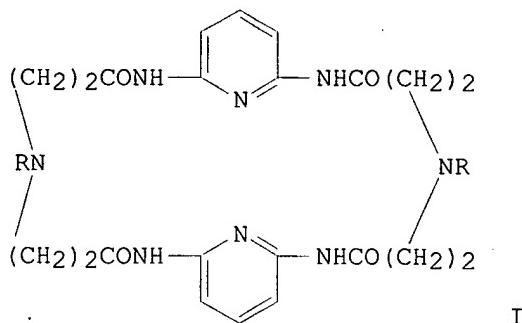
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CMF C22 H20 N4 O2

CM 2

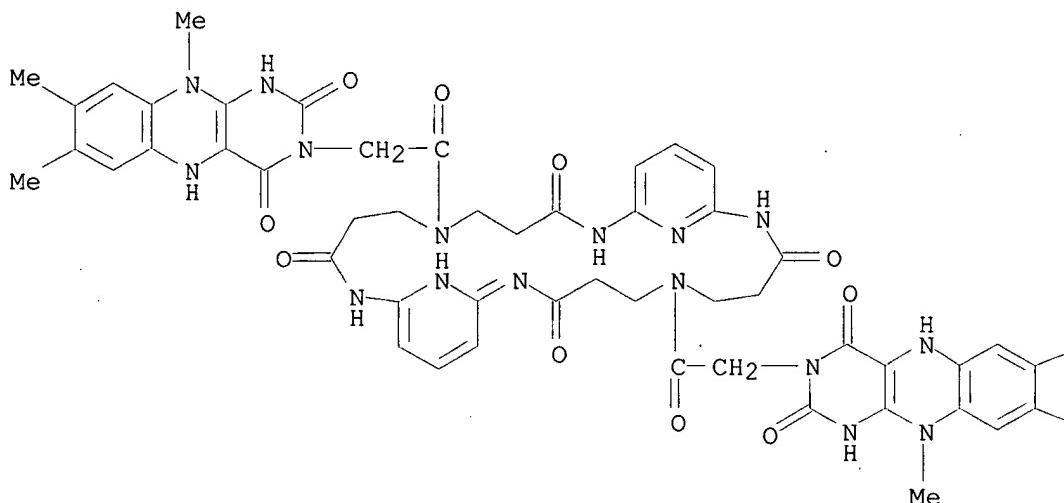
CRN 1075-49-6
CMF C9 H8 O2

L37 ANSWER 17 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1991:655534 CAPLUS
 DOCUMENT NUMBER: 115:255534
 TITLE: Molecular recognition of a pyrimidine dimer and
 photosensitized dimer splitting by a macrocyclic
 bis(diaminopyridine)
 AUTHOR(S): Goodman, M. Scott; Rose, Seth D.
 CORPORATE SOURCE: Dep. Chem. Biochem., Arizona State Univ., Tempe, AZ,
 85287-1604, USA
 SOURCE: J. Am. Chem. Soc. (1991), 113(24), 9380-2
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



- AB H-bonded mol. assocn. of macrocycle I (R = tosyl) with a pyrimidine photodimer (1,1'-dibutylthymine cis-syn-photodimer, II) was studied as a model for photorepair of pyrimidine dimers in DNA by photolyases. The assocn. const. of the 1:1 I:II complex was 1.5 .+-. 0.4 .times. 10⁴ M⁻¹. I [R = Me(CH₂)₂CO, indolylbutanoyl] photosensitized the splitting of dimer II, with the former functioning photocatalytically.
- IT 137126-44-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, and inactivity of, as photosensitizer for pyrimidine dimer
 photosplitting)
- RN 137126-44-4 CAPLUS
- CN 2,6,10,16,20,24,29,30-Octaazatricyclo[23.3.1.111,15]triaconta-
 1(29),11,13,15(30),25,27-hexaene-3,9,17,23-tetrone, 6,20-bis[(1,4,5,10-
 tetrahydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-
 (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

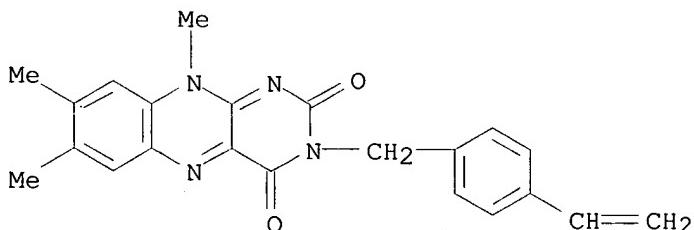
— Me
— Me

L37 ANSWER 18 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1991:602256 CAPLUS
 DOCUMENT NUMBER: 115:202256
 TITLE: An electrochemically prepared composite of polypyrrole and a flavin-containing polyanion; use as a biosensor
 AUTHOR(S): Schoo, H. F. M.; Challa, G.
 CORPORATE SOURCE: Lab. Polym. Chem., Univ. Groningen, Groningen, 9747 AG, Neth.
 SOURCE: Polym. Mater. Sci. Eng. (1991), 64, 300-1
 CODEN: PMSEDG; ISSN: 0743-0515
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The use is described of a polyanionic dopant, contg. covalently bound flavin moieties, in the prepn. of a catalytically active electrode and its application as a biosensor. Oxidn. of 1-benzyl-1,4-dihydronicotinamide was used as a model reaction.
 IT 136951-09-2
 RL: ANST (Analytical study)

(catalytically active electrode contg.)
 RN 136951-09-2 CAPLUS
 CN Benzoic acid, 4-ethenyl-, polymer with 3-[(4-ethenylphenyl)methyl]-7,8,10-trimethylbenzo[g]pteridine-2,4(3H,10H)-dione (9CI) (CA INDEX NAME)

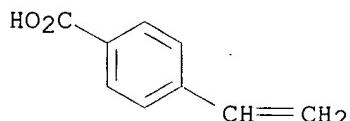
CM 1

CRN 136951-08-1
 CMF C22 H20 N4 O2

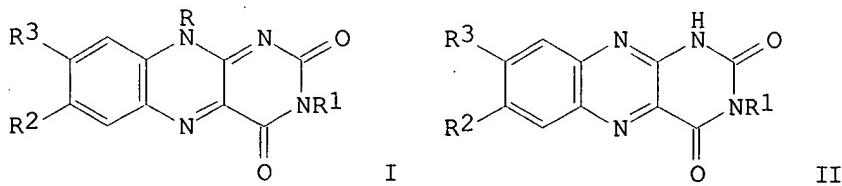


CM 2

CRN 1075-49-6
 CMF C9 H8 O2



L37 ANSWER 19 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1991:492221 CAPLUS
 DOCUMENT NUMBER: 115:92221
 TITLE: Synthesis of alloxazine derivatives by dealkylation of isoalloxazines at N-10
 Koziol, Jacek
 AUTHOR(S):
 CORPORATE SOURCE: Inst. Commod. Sci., Acad. Econ., Poznan, 60-967, Pol.
 SOURCE: Bull. Pol. Acad. Sci., Chem. (1991), 39(1), 37-9
 CODEN: BPACEQ; ISSN: 0239-7285
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 115:92221
 GI



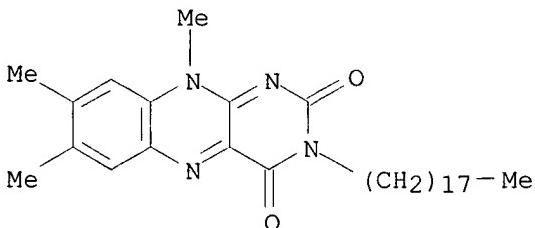
AB Refluxing of isoalloxazines e.g., I [R = Me, 1-D-ribityl; R1 = H, Me, undecyl, octadecyl; R2, R3 = H, Me] in several solvents and also in urea leads to dealkylation at N-10, allowing a simple synthesis of alloxazines II suitably substituted at N-3. Best results were obtained by heating isoalloxazines in the urea DMF mixt. and this method was successfully applied for the synthesis of 3-undecylumichrome.

IT 53965-14-3 73057-72-4

RL: RCT (Reactant)
(demethylation of)

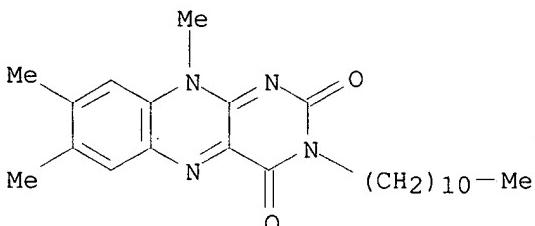
RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
(CA INDEX NAME)



RN 73057-72-4 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-undecyl- (9CI)
(CA INDEX NAME)



L37 ANSWER 20 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:453128 CAPLUS

DOCUMENT NUMBER: 111:53128

TITLE: Mechanism of mercury(II) reductase and influence of ligation on the reduction of mercury(II) by a water soluble 1,5-dihydroflavin

AUTHOR(S): Gopinath, Enona; Kaaret, Thomas W.; Bruice, Thomas C.

CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, 93116, USA

SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1989), 86(9), 3041-4
CODEN: PNASA6; ISSN: 0027-8424

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The nature and rate of redn. of Hg²⁺ to Hg⁰ by 1,5-dihydro-3-(3-sulfopropyl)lumiflavin (FIH₂) in buffered aq. soins. (pH 4.7) is dependent on the ligation of Hg²⁺. In the presence of N,N-bis(2-hydroxyethyl)glycine or when ligated to EDTA, the redn. is 1st-order in Hg²⁺ and FIH₂. The apparent 2nd-order rate const. with N,N-bis(2-hydroxyethyl)glycine (2.2 .times. 106M⁻¹ s⁻¹) is much greater than that in the presence of ligating EDTA (1.5 .times. 102M⁻¹ s⁻¹). When ligated by mercaptoethanesulfonate, redn. of Hg²⁺ by FIH₂ is characterized by a pronounced lag phase, which is dependent on the concn. of mercaptoethanesulfonate. The rate decreases with increase in

mercaptoethanesulfonate, and with an excess of 10 equiv, Hg²⁺ is not reduced by FIH₂. Bis-ligation by thiolate greatly decreases the reducibility of Hg²⁺ and further ligation by thiolate further retards the reaction. Comparison of oxidn.-redn. potentials at various pH values show that bis-ligation (or greater) of Hg²⁺ by thiolate substantially lowers the redn. potential of Hg²⁺ below that of 3-(3-sulfopropyl)lumiflavin (FLox). Thus, the ease of redn. of Hg²⁺ complexes by FIH₂ decreases with increasing thermodn. stability of the complex. These results do not support the proposed role of the thiol functionalities in facilitating the mercury(II) reductase (EC 1.16.1.1)-catalyzed redn. of Hg²⁺ through tris- or tetralligation of Hg²⁺.

IT

91385-12-5

RL: BIOL (Biological study)

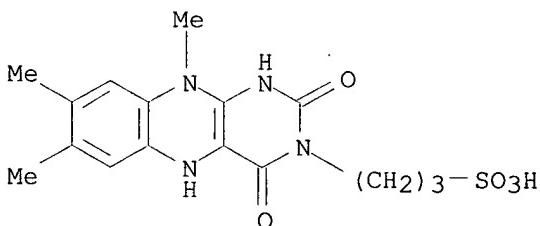
(mercury(II) redn. by, metal ligation effect on kinetics of,
mercury(II) reductase mechanism in relation to)

RN

91385-12-5 CAPLUS

CN

Benzo[g]pteridine-3(2H)-propanesulfonic acid, 1,4,5,10-tetrahydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



L37 ANSWER 21 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:146424 CAPLUS

DOCUMENT NUMBER: 110:146424

TITLE: An ODMR study of amphiphilic flavins in a Shpol'skii matrix

AUTHOR(S): Schlyer, B. D.; Maki, A. H.; Visser, A. J. W. G.

CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA

SOURCE: Chem. Phys. Lett. (1989), 154(1), 39-44

CODEN: CHPLBC; ISSN: 0009-2614

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Optical detection of triplet-state magnetic resonance was used to characterize the triplet states of N3-undecyllumiflavin (I), N3-undecyldeazalumiflavin (II), and N3-undecyllumichrome (III) which produce narrow-line Shpol'skii phosphorescence and ODMR in a crystal of decane. I and II have smaller zero-field splittings than III due to lower electron localization in III. The shorter triplet state lifetime of I in contrast to II is consistent with an important spin-orbit-coupling contribution of N5.

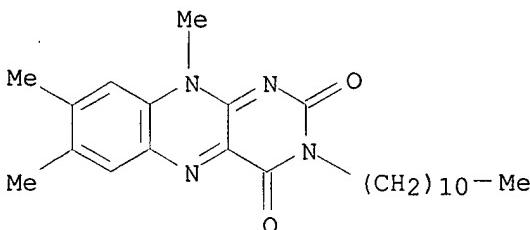
IT **73057-72-4**, N3-Undecyllumiflavin

RL: PRP (Properties)

(optically detected magnetic resonance of triplet state of)

RN 73057-72-4 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-undecyl- (9CI)
(CA INDEX NAME)



L37 ANSWER 22 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:18790 CAPLUS

DOCUMENT NUMBER: 108:18790

TITLE: Static and time-resolved fluorescence of an

AUTHOR(S): amphiphilic flavin in aerosol OT reversed micelles
Visser, Antonie J. W. G.; Vos, Kees; Santema, Jillert S.; Bouwstra, Jan; Van Hoek, Arie

CORPORATE SOURCE: Dep. Biochem., Agric. Univ., Wagerr

SOURCE: . Neth. Photochem. Photobiol. (1987), 46(4), 457-61

CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal

LANGUAGE: English

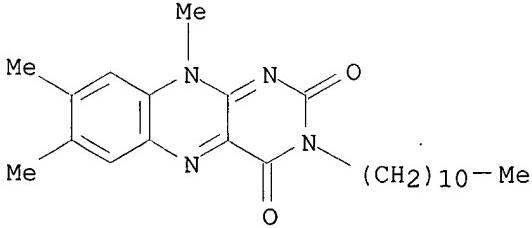
AB Spectral and time-resolved fluorescence studies have been carried out on N(3)-undecyllumiflavin dispersed in reversed micelles composed of the surfactant Na di(2-ethylhexyl)sulfosuccinate (Aerosol OT, AOT), various amounts of water and n-heptane as continuous phase. The fluorescence spectral properties (spectral distribution, quantum efficiencies and lifetimes) as function of the water to AOT molar ratio suggest that the flavin occupies a position within the surfactant boundary layer in close contact with water. The fluorescence anisotropy exhibits biexponential decay with a short (0.3 ns) and a longer (1.6-2.4 ns) correlation time. The contribution of the short component increases with the growth of the droplet, providing evidence for enhanced flexibility of the flavin in the interfacial layer.

IT 73057-72-4

RL: PRP (Properties)
(fluorescence of, in Aerosol OT reversed micelles)

RN 73057-72-4 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-undecyl- (9CI)
(CA INDEX NAME)



L37 ANSWER 23 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:501261 CAPLUS

DOCUMENT NUMBER: 103:101261

TITLE: 8-Azidoflavins as photoaffinity labels for flavoproteins

AUTHOR(S): Fitzpatrick, Paul F.; Ghisla, Sandro; Massey, Vincent
CORPORATE SOURCE: Dep. Biol. Chem., Univ. Michigan, Ann Arbor, MI,

SOURCE: 48109, USA
 J. Biol. Chem. (1985), 260(14), 8483-91
 CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal
 LANGUAGE: English

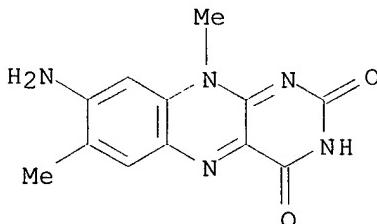
AB 8-Azidoflavins were synthesized and their potential as photoaffinity labels for flavoproteins was explored. They are very photolabile, and in aq. media they react with solvent to yield 8-aminoflavins and 8-hydroxylaminoflavins as the main products. They fulfill the criteria expected of a good photoaffinity label, since they bind stoichiometrically at the flavin-binding site of flavoproteins, thus minimizing problems of nonspecific labeling. Second, they absorb strongly in the visible, so that the reactive nitrene can be generated without short wavelength light, minimizing the possibility of light-induced damage of the protein. Third, in the absence of light, 8-azidoflavins are stable, permitting a study of their binding to apoproteins. 8-Azidoflavins were bound to hen egg white riboflavin-binding protein, *Megasphaera elsdenii* flavodoxin, yeast Old Yellow Enzyme, *Aspergillus niger*, glucose oxidase, and pig kidney D-amino acid oxidase, and the effect of exposure to visible light was detd. Only small exts. of covalent attachment of the flavin to the protein were found with flavodoxin, D-amino acid oxidase, and Old Yellow Enzyme; much more extensive labeling was obtained with glucose oxidase and riboflavin-binding protein. In addn. to their photoreactivity, 8-azidoflavins were converted to 8-aminoflavins by reaction with sulfite or upon redn. Similar reactions occur with 8-hydroxylamino-, 8-(O-methyl)hydroxylamino-, and 8-hydrazinoflavins, which serve as models for possible flavin-protein covalent linkages which could be formed in the photolabeling procedure. Some of the properties of these flavins, which were obtained by reaction of 8-F-flavin with the corresponding nucleophiles, are also described.

IT 3942-96-9

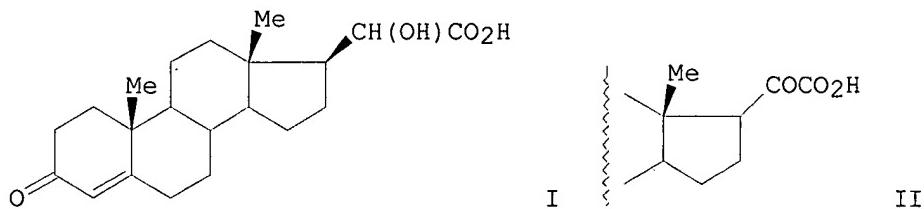
RL: PRP (Properties)
 (spectral properties of)

RN 3942-96-9 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



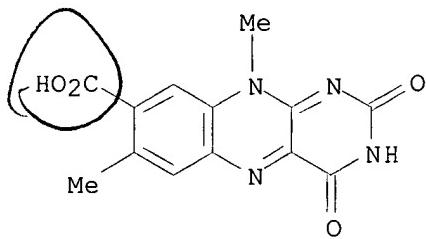
L37 ANSWER 24 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1986:186703 CAPLUS
 DOCUMENT NUMBER: 104:186703
 TITLE: Oxidation of corticosteroids by flavins
 AUTHOR(S): Jasiczak, J.; Smoczkiewicz, M. A.
 CORPORATE SOURCE: Inst. Commodity Sci., Acad. Econ., Poznan, 60 967, Pol.
 SOURCE: Tetrahedron Lett. (1985), 26(42), 5221-4
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 104:186703
 GI



AB Photolysis of deoxycorticosterone in an aq. alk. soln. (pH 9-11) contg. lumiflavin, 3-methylumiflavin, or 8-carboxylumiflavin gave the carboxylic acids I and II. Prednisolone, 9-fluoro-16.alpha.-hydroxyhydrocortisone (III), and the acetonide of III underwent analogous C-21 oxidn. reactions.

IT 101750-71-4
 RL: RCT (Reactant)
 (photochem. oxidn. by, of corticosteroids)

RN 101750-71-4 CAPLUS
 CN Benzo[g]pteridine-8-carboxylic acid, 2,3,4,10-tetrahydro-7,10-dimethyl-2,4-dioxo- (6CI, 9CI) (CA INDEX NAME)



L37 ANSWER 25 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1984:529998 CAPLUS
 DOCUMENT NUMBER: 101:129998
 TITLE: On the mechanism of flavin-catalyzed dehydrogenation .alpha.,.beta. to an acyl function. The mechanism of 1,5-dihydroflavin reduction of maleimides
 AUTHOR(S): Venkataram, U. V.; Bruice, Thomas C.
 CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, 93106, USA
 SOURCE: J. Am. Chem. Soc. (1984), 106(19), 5703-9
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Redn. of maleimide and its N-Me deriv. (I) by 1,5-dihydro-3-(3-sulfopropyl)lumiflavin (FlH₂) to give oxidized flavin (Flox) and succinimides is biphasic. The 1st phase involves general acid-assisted nucleophilic attack of FlH⁻ on the maleimide to yield 4a-substituted 4a,5-dihydroflavin covalent adducts. The Broensted .alpha. for the general-acid catalysis is -0.1 to -0.2. This observation would be expected for a Michael addn. of FlH⁻ on I to yield an unstable anionic 4a-adduct, which is trapped by proton transfer from general-acid species. The decompr. rate of the intermediate to yield Flox and succinimide is not measurably dependent on the concn. of general-base species. The reaction was 1st order in [HO⁻]. A mechanism involving preequil. ionization of the N(5)-H, followed by elimination of succinimide anion (specific-base catalysis) and formation of Flox, would require that the pKa for dissociation of the aniline-like N(5)-H is <23 in order that the elimination rate from

the anion does not exceed that for the vibration of the C-C bond that is broken. The HO--catalyzed elimination represents a concerted process with a Broensted .beta. approaching 1.0. The results of this study and the principle of microscopic reversibility are used to construct the mechanism of N-methylsuccinimide anion oxidn. by Flox to yield maleimide and FlH-. The possible implications of this mechanism for that of such dehydrogenating flavoenzymes as succinic acid dehydrogenase, fumarate reductase, acyl-CoA dehydrogenase, and acyl-CoA oxidase are considered.

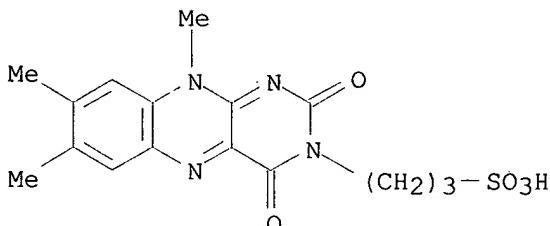
IT 36469-13-3

RL: RCT (Reactant)

(oxidn. by, of methylsuccinimide anion, mechanism of)

RN 36469-13-3 CAPLUS

CN Benzo[g]pteridine-3(2H)-propanesulfonic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



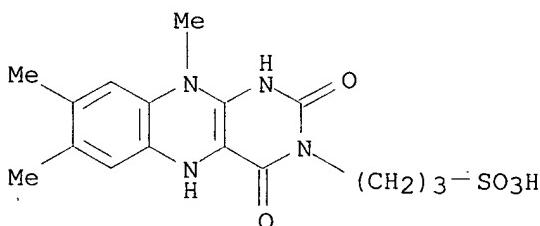
IT 91385-12-5

RL: RCT (Reactant)

(redn. by, of maleimides, mechanism of)

RN 91385-12-5 CAPLUS

CN Benzo[g]pteridine-3(2H)-propanesulfonic acid, 1,4,5,10-tetrahydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



L37 ANSWER 26 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1984:63982 CAPLUS

DOCUMENT NUMBER:

100:63982

TITLE:

Fluid solution and solid-state electron nuclear double resonance studies of flavin model compounds and flavoenzymes

AUTHOR(S):

Kurreck, H.; Bock, M.; Bretz, N.; Elsner, M.; Kraus, H.; Lubitz, W.; Mueller, F.; Geissler, J.; Kroneck, P. M. H.

CORPORATE SOURCE:

Inst. Org. Chem., Freie Univ. Berlin, Berlin, 1000/33, Fed. Rep. Ger.

SOURCE:

J. Am. Chem. Soc. (1984), 106(3), 737-46

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Partially deuterated and various substituted flavin and thiaflavin model compds. were synthesized. For the 1st time, high-resoln. H-, D-, and ¹⁴N-ENDOR and TRIPLE resonance expts. in fluid solns. were performed on

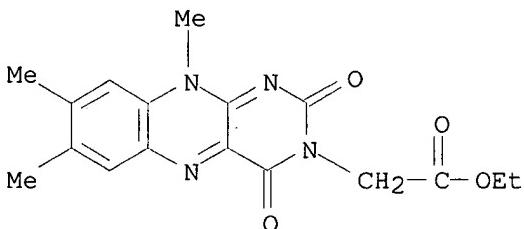
the paramagnetic derivs. of these compds. Addnl., valuable information was obtained about hyperfine anisotropies and mol. structures from ENDOR in rigid matrixes. Solid matrix ENDOR studies of native flavoenzymes, namely, Old Yellow enzyme (NADPH dehydrogenase), 2 flavodoxins, and a methanol oxidase are reported. The ENDOR matrix signals of the various flavoproteins were different in intensity, suggesting that the microenvironments are markedly different. Applicabilities and limitations of the ENDOR technique in the studies of flavins and flavoenzymes are discussed.

IT 74178-39-5

RL: BIOL (Biological study)
(ENDOR of)

RN 74178-39-5 CAPLUS

CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (7CI, 9CI) (CA INDEX NAME)



L37 ANSWER 27 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:98597 CAPLUS

DOCUMENT NUMBER: 100:98597

TITLE: The thermodynamics of flavin binding to the apoflavodoxin from Azotobacter vinelandii

AUTHOR(S): Carlson, Rick; Langerman, Neal

CORPORATE SOURCE: Dep. Chem. Biochem., Utah State Univ., Logan, UT, 84322, USA

SOURCE: Arch. Biochem. Biophys. (1984), 229(2), 440-7

CODEN: ABBIA4; ISSN: 0003-9861

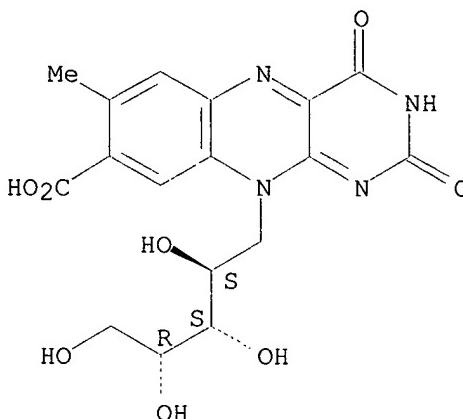
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A thermodn. study of the binding of flavins (FMN, FAD, 8-carboxylic acid riboflavin) to the purified apoflavodoxin from *A. vinelandii* was conducted. The binding of FMN was studied at a no. of temps. (10, 15, 20, 25, and 30.degree.), pHs (6.0, 7.4, and 9.0), and buffer conditions. The binding of FAD was studied at pH 7.4 and 25.degree. under a no. of buffer conditions. The binding of 8-carboxylic acid riboflavin to the apoflavodoxin and the binding of FMN to the dimeric form of the apoflavodoxin were investigated at pH 7.4 and 25.degree.. Enthalpies of binding for FMN, FAD, and 8-carboxylic acid riboflavin were -28.3, -16.6, and -14.0 kcal/mol, resp. The enthalpy of binding of FMN to the dimeric form of the apoflavodoxin was -22.2 kcal/mol of binding sites. Binding consts. of .apprx.108, 106, and 106 were obtained for the binding of FMN, FAD, and 8-carboxylic acid riboflavin, resp. By using established thermodn. relations, free energy and entropy changes were calcd. The entropy data indicate that a large degree of ordering of the system occurs on flavin binding. The pH data suggest that FMN may bind in both the mono- and dianion forms, and that binding does not change the pKa of any functional group in the system. The phosphate group is apparently responsible for the binding enthalpy obsd. for the binding of FMN. The temp.-dependence data over the temp. range studied is biphasic, centered at 20.degree., indicating that flavin binding to the protein occurs in 2 thermodn. states corresponding to the 2 heat capacities obsd. A model for flavin binding is discussed.

IT 28083-73-0
 RL: BIOL (Biological study)
 (apoflavodoxin binding of, thermodn. of)
 RN 28083-73-0 CAPLUS
 CN Riboflavin, 8-carboxy-8-demethyl- (9CI) (CA INDEX NAME)

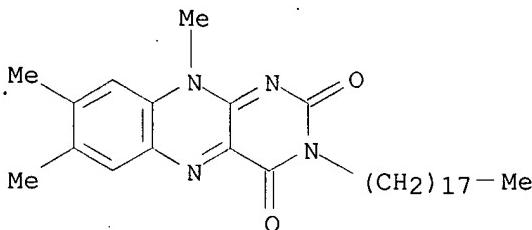
Absolute stereochemistry.



L37 ANSWER 28 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1985:57897 CAPLUS
 DOCUMENT NUMBER: 102:57897
 TITLE: Bluelight-induced, flavin-mediated transport of redox equivalents across artificial bilayer membranes
 AUTHOR(S): Schmidt, Werner
 CORPORATE SOURCE: Fak. Biol., Univ. Konstanz, Konstanz, D-7750/1, Fed.
 Rep. Ger.
 SOURCE: J. Membr. Biol. (1984), 82(2), 113-22
 CODEN: JMBBBO; ISSN: 0022-2631

DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Physicochem. properties of vesicle-bound flavins were studied. An advanced model system was designed to study the mechanisms underlying blue light-induced redox transport across artificial membranes. The lumen of single-shelled vesicles was charged with cytochrome c, and an amphiphilic flavin (AF1 3, AF1 10) was bound to the membrane. Upon irradn. with blue light, redox equivs. are translocated from exogenous 1e- (EDTA) and 2e- (BH3CN-) donors across the membrane, reducing the trapped cytochrome c under both aerobic and anaerobic conditions. The mechanisms are explored and evidence for the involvement of various redox states of O, dihydroflavin, and flavosemiquinone is presented.

IT 53965-14-3
 RL: BIOL (Biological study)
 (redox equiv. transport by, in liposomes, blue light stimulation of)
 RN 53965-14-3 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI) (CA INDEX NAME)



L37 ANSWER 29 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:19565 CAPLUS

DOCUMENT NUMBER: 100:19565

TITLE: Further photophysical and photochemical characterization of flavins associated with single-shelled vesicles

AUTHOR(S): Schmidt, Werner

CORPORATE SOURCE: Fak. Biol., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.

SOURCE: J. Membr. Biol. (1983), 76(1), 73-82

CODEN: JMBBBO; ISSN: 0022-2631

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A detailed anal. of the Sepharose 4B elution profile of various sonicated phospholipids demonstrates the presence of 3 distinct particle populations. Electron microscopy reveals heterogeneous multilamellar lipid aggregates of a diam. >500 .ANG. diam. in fraction II, and previously unreported micellar structures of .apprx.50 .ANG. diam. in fraction III. Fraction II vesicles are very similar to those obtained by the deoxycholate procedure. Fine structure anal. of cor. fluorescence and fluorescence polarization spectra of amphiphilic 7,8,10-trimethyl-3-octadecylisoalloxan (AFl 3) bound to vesicles prep'd. from various phospholipids demonstrates the specificity of the flavin-membrane interaction. When bound to fraction I, II, and III of sonicated egg lecithin, AFl 3 exhibits different temp. (i.e. phase) dependencies. Flavin-membrane interaction thus depends strongly upon the particular lipid structure as well as the lipid compn. The excited state of flavin involved in photochem. and photophys. reactions (triplet or singlet) is identified. Finally, the dependence of the photoreactions of vesicle-assocd. flavins on parameters such as pH, temp., and ionic strength are discussed. Comparison of photoreactions of isotropic and anisotropic flavins suggests possible mechanisms.

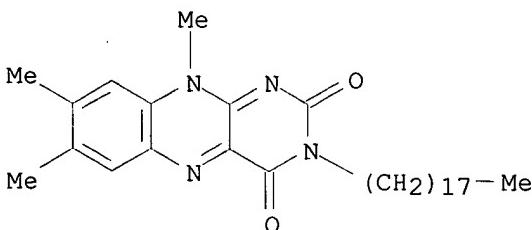
IT 53965-14-3

RL: BIOL (Biological study)

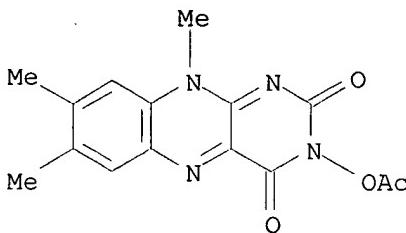
(photochem. and photophysics of, in liposomes, pH and temp. in relation to)

RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
(CA INDEX NAME)



L37 ANSWER 30 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1982:419323 CAPLUS
 DOCUMENT NUMBER: 97:19323
 TITLE: The binding of flavin derivatives to the riboflavin-binding protein of egg white. A kinetic and thermodynamic study
 AUTHOR(S): Becvar, James; Palmer, Graham
 CORPORATE SOURCE: Biophys. Res. Div., Univ. Michigan, Ann Arbor, MI, 48103, USA
 SOURCE: J. Biol. Chem. (1982), 257(10), 5607-17
 CODEN: JBCHA3; ISSN: 0021-9258
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A method is described for the prepn. and isolátion of a riboflavin-binding protein in gram quantity. The product is homogeneous in size and in binding character, but slightly heterogeneous in net charge; it consists of a single polypeptide chain of .apprx.30,000 daltons when examd. by SDS gel electrophoresis. An affinity chromatog. method is described by which flavin analogs and impurities can be sepd. on G-50 Sephadex. Aporiboflavin-binding protein complexes a variety of flavin analogs with >95% quenching of flavin fluorescence. One mol of aporiboflavin-binding protein contains 1 mol of riboflavin binding sites. The other flavin analogs also bind with 1:1 stoichiometry. Van't Hoff analyses for binding to aporiboflavin-binding protein of >20 flavin analogs at pH 7.0 are linear over the temp. range 10-40.degree.. Equil. binding energies lie in the ranges: .DELTA.Gu from -7 to -15 kcal/mol, .DELTA.H from -13 to -20 kcal/mol, and .DELTA.Su from -3 to -34 entropy units (e.u.)/mol. Several sites on the flavin are important to binding, although no 1 site dominates the interaction. The kinetics of flavin binding to aporiboflavin-binding protein were examd. by stopped flow fluorimetry. The quenching of the flavin fluorescence is accurately described by a unique 2nd order rate const. under a variety of conditions, demonstrating that the quenching process monitors the assocn. reaction. Assocn. rate consts. approaching 3 .times. 10⁸ M⁻¹ s⁻¹ are obsd. for binding of flavin analogs to aporiboflavin-binding protein at 25.degree. and pH 7.0. Arrhenius analyses are linear over 10-40.degree. range, and yield activation energies for flavin analog binding which lie in the ranges: .DELTA.Gu.++ from 3.5 to 5.5 kcal/mol, .DELTA.H.++ from 4.5 to 8 kcal/mol, and .DELTA.Su.++ from -2 to +12 e.u./mol. The relaxation kinetics for the dissochn. of several analog-apoprotein complexes were examd. at several temps. For most complexes, the binding process is adequately described by a single step equil., allowing the dissochn. rate consts. for the complexes to be calcd. from the equil. and assocn. rate consts. Because the variation in the magnitude of the assocn. rate const. is much less than the variation in the equil. consts., it is concluded that the dissochn. process dets. the strength of the interaction.
 IT 75016-33-0
 RL: BIOL (Biological study)
 (riboflavin-binding protein of egg white binding of, thermodn. of)
 RN 75016-33-0 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-(acetoxy)-7,8,10-trimethyl- (9CI)
 (CA INDEX NAME)



L37 ANSWER 31 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:13852 CAPLUS

DOCUMENT NUMBER: 98:13852

TITLE: Application of an improved spectroelectrochemical cell to the study of the redox properties of lumiflavin 3-acetate, tetraammine ruthenium(II) 10-methylisoalloxazine, and 5-deazaflavin

AUTHOR(S): Condit, David; Stankovich, Marian

CORPORATE SOURCE: Dep. Chem., Univ. Massachusetts, Amherst, MA, USA

SOURCE: Dev. Biochem. (1982), 21(Flavins Flavoproteins), 528-32

CODEN: DEBIDR; ISSN: 0165-1714

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An improved spectroelectrochem. cell is described, and the improved cell was tested by reductive titrn. of lumiflavin-3-acetate (I), 5-deazaflavin (II), and Ru(II)-10-methylisoalloxazine (III) complex under anaerobic conditions. The major improvements consisted of replacing the glass stirrer with a polyethylene-encased magnetic stirrer for more efficient stirring and coating the Au-wire working electrode with Hg to extend its neg. potential limit. Reductive titrn. of I was carried out by using Me viologen (MV) and 4,4'-dimethyl-1,1'-trimethylene-2,2'-dipyridinium bromide (IV) as mediator dyes, and electrons were transferred to I rapidly and with 100% current efficiency by both mediators. Redn. of II with IV as the mediator dye under a variety of anaerobic gave 2-product mixts., and electron transfer between the 2 species was slow. A current efficiency of 91-94% was obtained by reductive titrn. of Ru(II)-III complex.

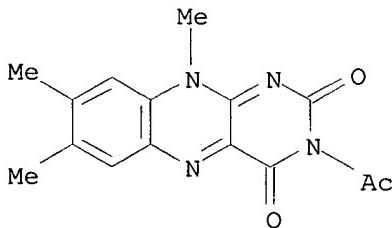
IT 60823-53-2

RL: PRP (Properties)

(redox properties of, spectroelectrochem. cell for study of)

RN 60823-53-2 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-acetyl-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



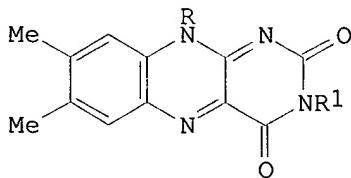
L37 ANSWER 32 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:29992 CAPLUS

DOCUMENT NUMBER: 98:29992

TITLE: Limited rotational motion of amphiphilic flavins in

AUTHOR(S): dipalmitoylphosphatidylcholine vesicles
 Visser, A. J. W. G.
 CORPORATE SOURCE: Dep. Biochem., Agric. Univ., Wageningen, 6703 BC,
 Neth.
 SOURCE: Biochim. Biophys. Acta (1982), 692(2), 244-51
 DOCUMENT TYPE: CODEN: BBACAO; ISSN: 0006-3002
 LANGUAGE: English
 GI



I, R=Me, R₁=(CH₂)₁₇Me
 II, R=(CH₂)₁₇Me, R₁=H

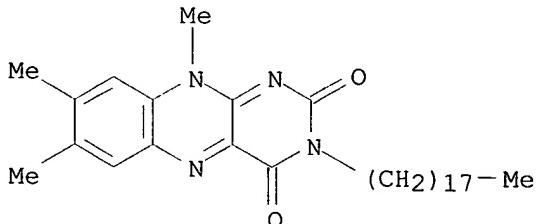
AB The rotational motion of amphiphilic flavins I and II in dipalmitoylphosphatidylcholine bilayers was investigated with fluorescence anisotropy decay measurements. At temps. of 10-50.degree. the rotation was anisotropic, which indicated composite motion of both the aliph. side chain and the isoalloxazine moiety of the octadecyllumiflavin derivs. Above the phase transition temp. (cryst..fwdarw.liq.-cryst. state) the depolarization was complete within the av. flavin fluorescence lifetime, implicating unrestricted motion and resulting in a nonordered microenvironment. In the gel or cryst. state the flavin motion was best characterized as a limited rotation or librational motion. The fluorescence decay of the flavins was heterogeneous at temps. of 10-50.degree., which was explained by assuming nanosecond relaxation of the polar phosphatidyl head groups around the excited flavin. The lack of a significant cholesterol effect suggested that the isoalloxazine was located at the interphase of the bilayer and not in the hydrocarbon region. The microstructure was fluidlike, not in agreement with a preferred static localization of the flavins in the bilayer.

IT 53965-14-3

RL: BIOL (Biological study)
 (rotation of, in dipalmitoylphosphatidylcholine liposomes)

RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
 (CA INDEX NAME)



L37 ANSWER 33 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1981:475696 CAPLUS
 DOCUMENT NUMBER: 95:75696
 TITLE: Molecular complex of lumiflavin and 2-aminobenzoic

AUTHOR(S): Shieh, Huey-Sheng; Ghisla, Sandro; Hanson, Louise Karle; Ludwig, Martha L.; Nordman, Christer E.

CORPORATE SOURCE: Dep. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA

SOURCE: Biochemistry (1981), 20(16), 4766-74

DOCUMENT TYPE: Journal

LANGUAGE: English

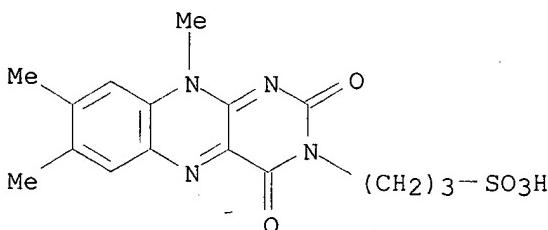
AB The mol. complex lumiflavin.cntdot.2-aminobenzoic acid monohydrate ($C_{13}H_{12}N_4O_2 \cdot C_7H_7NO_2 \cdot H_2O$) crystallizes from aq. soln. as red triclinic prisms. The space group is P.hivin.1 with cell dimensions $a = 9.660$, $b = 14.866$, $c = 7.045$.ANG., $\alpha = 95.44$, $\beta = 95.86$, and $\gamma = 105.66$.degree.. The crystal structure was solved by direct methods and refined by block-diagonal least-squares procedures to an R value of 0.050 on the basis of 1338 obsd. reflections. The structure is composed of stacks of alternating lumiflavin and unionized (neutral) 2-aminobenzoic acid mols. Two different modes of stacking interaction are obsd. In one mode, 2-aminobenzoic acid overlaps all 3 of the isoalloxazine rings, at a mean distance of 3.36 .ANG.; in the other, 2-aminobenzoic acid interacts with the pyrazine and dimethylbenzene moieties, at a distance of 3.42 .ANG.. Perpendicular to the stacking direction, the mols. form a continuous sheet. Each flavin is H-bonded via O-2 and NH-3 to 2 sym. related aminobenzoates; the water of crystn. forms 3 H bonds, bridging 2 flavins, via O-4 and N-5, and one aminobenzoic acid. The red color of the crystals results from a charge-transfer transition involving stacked flavin and 2-aminobenzoic acid mols. Measurements of the polarized optical absorption spectra of crystals show that the transition moment direction for the long wavelength absorbance (beyond 530 nm) contains an out-of-plane component which can only arise from a charge-transfer interaction. Since the amino N does not make exceptionally close interactions with isoalloxazine atoms in either stacking mode (min. interat. distances 3.52 .ANG.), the charge transfer is presumed to involved .pi. orbitals of the 2-aminobenzoic acid donor.

IT 36469-13-3

RL: PRP (Properties)
(absorption spectra of, lumiflavin-aminobenzoate complex in comparison with)

RN 36469-13-3 CAPLUS

CN Benzo[g]pteridine-3(2H)-propanesulfonic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



L37 ANSWER 34 OF 72 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:569137 CAPLUS
DOCUMENT NUMBER: 95:169137
TITLE: Substitution of the flavin chromophore with lipophilic side chains: a novel membrane redox label
AUTHOR(S): Michel, Heinrich; Hemmerich, Peter
CORPORATE SOURCE: Fac. Biol., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: J. Membr. Biol. (1981), 60(2), 143-53

CODEN: JMBBBO; ISSN: 0022-2631

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Amphiphilic flavins octadecylated in positions 3, 5, 7, 8 and 10 were prepd. 3-, 7-, And 10-amphiflavins were obtained by new total syntheses. Furthermore, 3-amphiflavin was obtained by octadecylation of natural flavin in the oxidized state, whereas dihydro-5-amphiflavin was obtained by alkylation under reducing conditions. In the course of these studies, a novel selective oxidn. reaction was obsd. at the 8-Me group of natural flavins. In this way lumiflavin and riboflavin derivs. could be converted directly to flavin-8-nor-8-carboxylic acids or the corresponding alkyl esters. The new flavin derivs. lend themselves to incorporation into lipid vesicles, for model studies of anisotropic flavin chem. and redox transfer through membranes. The new flavins are characterized by means of absorption, fluorescence, and proton NMR.

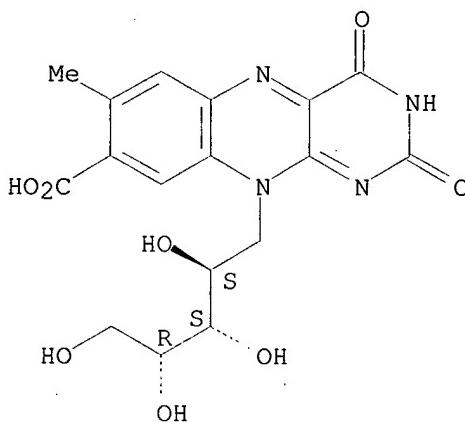
IT 28083-73-0P 53965-14-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

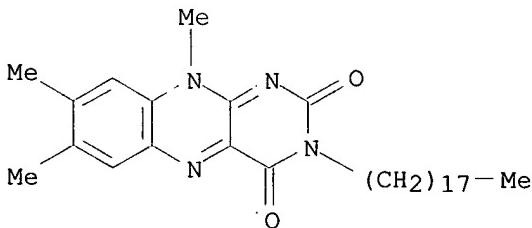
RN 28083-73-0 CAPLUS

CN Riboflavin, 8-carboxy-8-demethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
(CA INDEX NAME)

L37 ANSWER 35 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:492499 CAPLUS

DOCUMENT NUMBER: 95:92499

TITLE: On the redox reactions and accessibility of

amphiphilic flavins in artificial membrane vesicles

Schmidt, W.; Hemmerich, P.

AUTHOR(S): Dep. Biol., Univ. Konstanz, Konstanz, D-7750, Fed.

CORPORATE SOURCE:

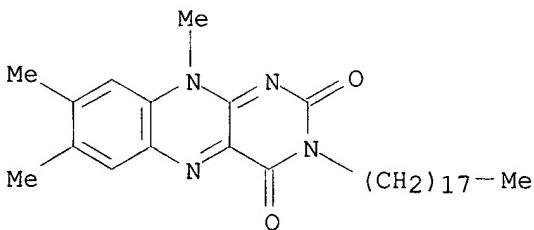
SOURCE: Rep. Ger.
 J. Membr. Biol. (1981), 60(2), 129-41
 CODEN: JMBBBO; ISSN: 0022-2631

DOCUMENT TYPE: Journal
 LANGUAGE: English

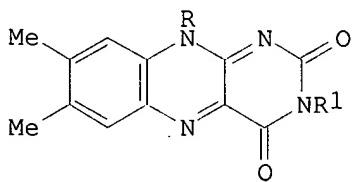
AB (Photo)redox reactions of different amphiphilic flavins bound to artificial membrane vesicles made from 3 different, satd. phospholipids were investigated and compared with those of isotropically dissolved flavin. By use of C18 hydrocarbon chains, substituted at different positions, the flavin nucleus can be specifically oriented within the membrane, thereby imposing sterically anisotropic environments, which are liable to control flavin (photo)chem. A spectrophotometric setup was designed, permitting photoredn. of flavin and its simultaneous control by fluorescence. The characteristic temp. dependency of the (vesicle-bound) flavin photoredn. by external and internal photosubstrates, as studied for the different lipid/flavin systems, is explained by the displacement of the flavin nucleus from the area of the polar head groups of the lipid into the more hydrophobic parts of the membrane upon phase transition (gel .fwdarw. liq. cryst.). Evidence is presented that this flavin displacement is correlated with the pre-phase transition rather than with the main phase transition, supporting a former hypothesis of the structural nature of the pre-phase transitions. The transport of redox equivs. across flavin-charged membranes is discussed. The accessibility of vesicle-bound flavins to a variety of exogenous ions (H+, Cs+, EDTA, NTA, BH3CN-, I-, N3-) is explored as a function of temp., i.e., membrane phase which, in turn, appears to control the permeability of the lipid/water interface. Therefore, it appears indispensable to include the interface as a sep. structural entity in any theory on membrane transport.

IT 53965-14-3
 RL: RCT (Reactant)
 (photoredn. of, in phospholipid liposome)

RN 53965-14-3 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
 (CA INDEX NAME)



L37 ANSWER 36 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1982:117757 CAPLUS
 DOCUMENT NUMBER: 96:117757
 TITLE: Preferred conformation of flavinyltryptophan peptides revealed by polarized excitation energy transfer
 Visser, A. J. W. G.; Santema, J. S.
 CORPORATE SOURCE: Dep. Biochem., Agric. Univ., Wageningen, 6703 BC, Neth.
 SOURCE: Photobiochem. Photobiophys. (1981), 3(2), 125-33
 CODEN: PHOPDS; ISSN: 0165-8646
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



- I, R=(CH₂)₄CO-Trp-OMe, R₁=Me
 II, R=Me, R₁=CH₂CO-Trp-OMe
 III, R=(CH₂)₄CO₂Me, R₁=Me
 IV, R=Me, R₁=CH₂CO₂Me

AB The flavylyltryptophan peptides I and II and flavin ref. compds. III and IV were studied with the objective of estg. orientation distribution. Polarized emission properties of the peptides and flavin ref. compds. were measured in propylene glycol at -50.degree. to minimize rotatory depolarization. In the spectral region where the tryptophanyl moiety absorbs light, the depolarization is larger than that obsd. in the flavin ref. compd. The addnl. depolarization is due to radiationless energy transfer from tryptophan to flavin. The measured depolarization was used to est. the relative orientation of the isoalloxazine and indole moieties.

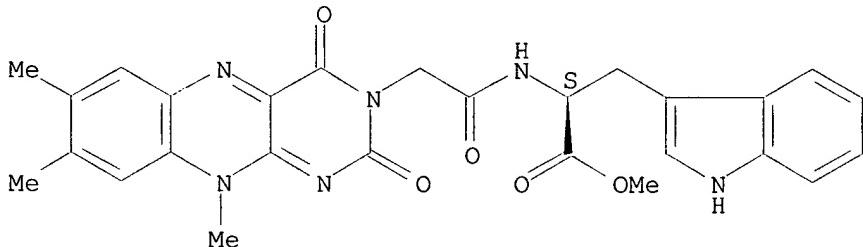
IT 21099-87-6

RL: BIOL (Biological study)
 (conformation and spectral properties of)

RN 21099-87-6 CAPLUS

CN L-Tryptophan, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

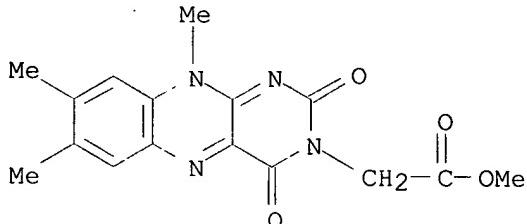


IT 81039-21-6

RL: BIOL (Biological study)
 (flavylyltryptophan in relation to)

RN 81039-21-6 CAPLUS

CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, methyl ester (9CI) (CA INDEX NAME).



L37 ANSWER 37 OF 72 CAPLUS COPYRIGHT 2002 ACS

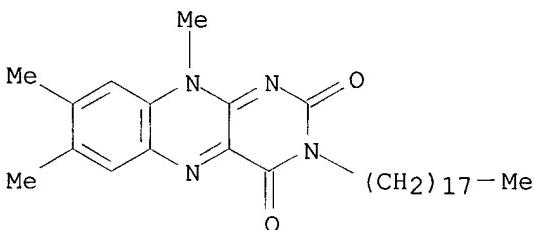
ACCESSION NUMBER: 1981:586194 CAPLUS

DOCUMENT NUMBER: 95:186194

TITLE: Fluorescence properties of isotropically and

AUTHOR(S): anisotropically embedded flavins
 Schmidt, Werner
 CORPORATE SOURCE: Fak. Biol., Univ. Konstanz, Konstanz, D-7750/1, Fed.
 Rep. Ger.
 SOURCE: Photochem. Photobiol. (1981), 34(1), 7-16
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The flavin photoprocesses in anisotropically phospholipid vesicle-bound flavins were studied by cor. fluorescence excitation and emission spectra. The flavin nucleus was variously anchored within the membrane/H₂O interface with aliph. C₁₈H₃₇ chains at positions N-3, C-7, and C-10, mimicking the various positions and microenvironments of the isoalloxazine ring in flavoproteins. The angles between the different electronic transition moments of isotropically dissolved or membrane-bound flavins were obtained from polarization spectra. Polarization and angle spectra of isotropically and various anisotropically embedded flavins show strong differences, reflecting the specific interaction with the matrixes. The radiative flavin-flavin interaction (selfcontact) on the membrane was detd. from the concn. dependence of fluorescence polarization.

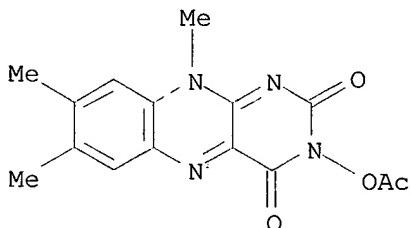
IT 53965-14-3
 RL: PRP (Properties)
 (vesicle-bound, fluorescence spectra of)
 RN 53965-14-3 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
 (CA INDEX NAME)



L37 ANSWER 38 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1980:599477 CAPLUS
 DOCUMENT NUMBER: 93:199477
 TITLE: Resonance Raman spectra of flavin derivatives containing chemical modifications in positions 7 and 8 of the isoalloxazine ring
 AUTHOR(S): Schopfer, Lawrence M.; Morris, Michael D.
 CORPORATE SOURCE: Dep. Biol. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA
 SOURCE: Biochemistry (1980), 19(21), 4932-5
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The resonance Raman spectra of riboflavin, 7,8-dichlororiboflavin, 8-chlororiboflavin, 8-bromoriboflavin, 8-(methylthio)riboflavin, 7-chlorolumiflavin, 8-norlumiflavin, 7,8-norlumiflavin, and 3-acetoxylumiflavin were measured in complexes with riboflavin-binding protein, which was used as a fluorescence quenching agent. Shifts in the positions of Raman bands in the vicinity of 1250, 1405, 1550, and 1585 cm⁻¹ were obsd. in the spectra of many of these flavin derivs. Comparable shifts were found in the IR spectra (solid KBr) of the uncomplexed flavins. The perturbed bands have been previously assigned to reasonably localized stretching modes in the isoalloxazine system, which are well removed from the 7 and 8 positions. Thus, a direct effect on these bands

due to modification of the substituents at positions 7 and 8 is precluded. These observations indicate that these Raman bands are assocd. with highly delocalized arom. framework vibrations.

- IT 75016-33-0D, riboflavin-binding protein complex
 RL: PRP (Properties)
 (resonance Raman spectrum of, delocalized arom. framework vibration in relation to)
- RN 75016-33-0 CAPLUS
- CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-(acetyloxy)-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 39 OF 72 CAPLUS COPYRIGHT 2002 ACS

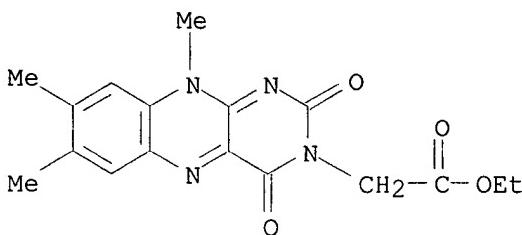
ACCESSION NUMBER: 1980:445605 CAPLUS
 DOCUMENT NUMBER: 93:45605
 TITLE: Distinction of 2e- and 1e- reduction modes of the flavin chromophore as studied by flash photolysis
 Hemmerich, Peter; Knappe, Wolfgang-R.; Kramer, Horst E. A.; Traber, Rainer
 CORPORATE SOURCE: Fachber. Biol., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
 SOURCE: Eur. J. Biochem. (1980), 104(2), 511-20
 CODEN: EJBCAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Evidence is given for the fact that the excited flavin triplet ($3\text{Fl}^*\text{ox}$) exhibits competitive 1- and 2-electron transfer chem., depending on the nature of the photosubstrate. The external 2e- donor borohydride competes effectively with the internal 1e- donors, namely excess starting flavin in the ground state (Flox) and, as primary product, (alkyl)dihydroflavin (RFlredH). Some of the flavin radicals, obsd. by earlier authors in the reaction of $3\text{Fl}^*\text{ox}$ with CH or CCO_2^- substrates or in the autophotolytic side-chain cleavage of riboflavin, are due to the dye-dye reaction: $3\text{Fl}^*\text{ox} + \text{Fl}\text{ox} \rightarrow \text{F}\text{ldarw. H}\text{f}\text{l.bul.} + \text{F}\text{l.bul.} \rightarrow \text{F}\text{ldarw. 2F}\text{lox.bul.}$. In contrast, flavin photoredn. by borohydride or hydrocarbon substrates need not involve radicals, but may in fact be a hydride or carbanion-plus-proton addn. towards the highly polar and considerably basic acceptor triplet. The products are much more photoreactive than the starting substrates, which leads to the secondary photocoproportionation: $3\text{Fl}^*\text{ox} + \text{RF}\text{lredH} \rightarrow \text{F}\text{ldarw. H}\text{f}\text{l.bul.} + \text{RF}\text{l.bul.}$ ($\text{R} = \text{H, alkyl}$). This latter reaction is the 2nd source of radicals in the system. This photohydrogenation of flavin is mechanistically related to the biol. redn. of flavin by CH substrates.

- IT 74178-39-5
 RL: RCT (Reactant)
 (photoredn. of)
- RN 74178-39-5 CAPLUS
- CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (7CI, 9CI) (CA INDEX NAME)



L37 ANSWER 40 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:437945 CAPLUS

DOCUMENT NUMBER: 95:37945

TITLE: Flavin-mediated photoreduction of nitrate by nitrate reductase of higher plants and microorganisms

AUTHOR(S): Zumft, W. G.; Castillo, F.; Hartmann, K. M.

CORPORATE SOURCE: Inst. Bot., Univ. Erlangen-Nuernberg, Erlangen, 8520, Fed. Rep. Ger.

SOURCE: Blue Light Syndr., [Proc. Int. Conf. Eff. Blue Light Plants Microorg.] (1980), Meeting Date 1979, 422-8.

Editor(s): Senger, Horst. Springer: Berlin, Fed. Rep. Ger.

DOCUMENT TYPE: Conference

LANGUAGE: English

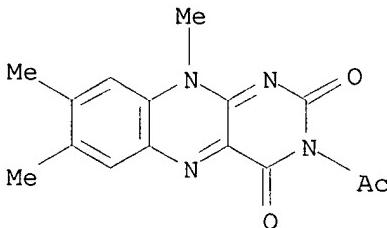
AB Photoredn. of riboflavin or FMN constituted an efficient electron donor system for a wide range of nitrate reductase. Kinetic characterization of this photochem. assay system by a Hill plot of the fluence effect (cor. to yield a function of the photon dose) gave a slope $n = 1.95$, confirming the flavin-mediated photocatalysis as being 2nd order. The overall quantum yield of the flavin-mediated photoredn. of nitrate at 448 nm was apprx. 0.03. Deazaflavins were nearly inactive as electron donors for nitrate reductase from 3 different organisms.

IT 60823-53-2

RL: BIOL (Biological study)
(nitrate reductase photocatalysis in presence of)

RN 60823-53-2 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-acetyl-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 41 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:402268 CAPLUS

DOCUMENT NUMBER: 95:2268

TITLE: Artificial flavin/membrane systems; a possible model for physiological blue light action

AUTHOR(S): Schmidt, W.

CORPORATE SOURCE: Biol. Inst., Univ. Konstanz, Konstanz, 7750, Fed. Rep. Ger.

SOURCE: Blue Light Syndr., [Proc. Int. Conf. Eff. Blue Light

Plants Microorg.] (1980), Meeting Date 1979, 212-20.
 Editor(s): Senger, Horst. Springer: Berlin, Fed. Rep. Ger.

DOCUMENT TYPE: Conference
 LANGUAGE: English

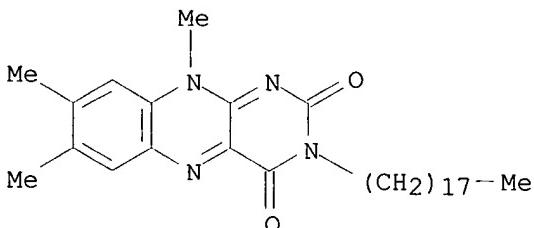
AB As a model of the blue light photoreceptor, 7,8,10-trimethyl-3-octadecylisoalloxazine, 3,8,10-trimethyl-7-octadecylisoalloxazine, 3,7,8-trimethyl-10-octadecylisoalloxazine, and 3-methyl-10-octadecylisoalloxazine were anchored in satd. lecithin liposomes. All the amphiphilic flavins bound in reasonable concns. (lipid/flavin, 100/1) and their orientation, localization, and mobility were controlled by the specific attachment of the hydrocarbon chain to the flavin and membrane phase. From fluorescence measurements on the models, the occurrence of 2 flavin moieties differing in microenvironment within the membrane is suggested. The flavins were highly immobilized on binding to the membranes, and the access of exogenous mols. to the flavin was largely diminished and depended on the charge of the mol. and the phase of the membrane. These model systems may be used to study anisotropic flavin chem.

IT 53965-14-3

RL: BIOL (Biological study)
 (lecithin liposome-anchored, as blue-light photoreceptor model)

RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
 (CA INDEX NAME)



L37 ANSWER 42 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:545088 CAPLUS

DOCUMENT NUMBER: 93:145088

TITLE: High-resolution fluorescence and excitation spectroscopy of N3-undecyllumiflavin in n-decane

AUTHOR(S): Plattenkamp, R. J.; Van Osnabrugge, H. D.; Visser, A. J. W. G.

CORPORATE SOURCE: Cent. Study Excited States Mol., Univ. Leyden, Leyden, Neth.

SOURCE: Chem. Phys. Lett. (1980), 72(1), 104-11
 CODEN: CHPLBC; ISSN: 0009-2614

DOCUMENT TYPE: Journal

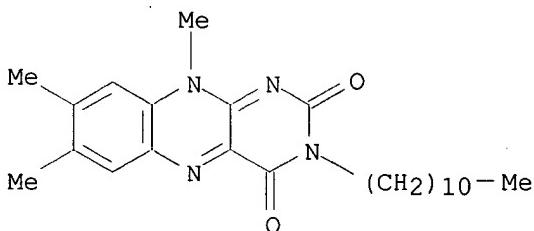
LANGUAGE: English

AB Lumiflavin derivs. with an undecyl tail on either N-3 or N-10 yield highly resolved fluorescence and absorption spectra in n-decane at 4.2 K. By site-selection techniques, single-site emission and excitation spectra were obtained (typical linewidths 5 cm⁻¹). The vibrational frequencies in the ground and 1st excited singlet states were nearly equal. The vibronic transitions were weak compared with the 0-0 transitions and it is concluded that the geometry of the 1st excited singlet state differs only slightly from that of the ground state.

IT 73057-72-4

RL: PRP (Properties)
 (fluorescence and absorption spectra of, in n-decane)

RN 73057-72-4 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-undecyl- (9CI)
 (CA INDEX NAME)



L37 ANSWER 43 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:633102 CAPLUS
 DOCUMENT NUMBER: 93:233102
 TITLE: The interaction of flavins with egg white
 riboflavin-binding protein
 AUTHOR(S): Choi, Jung-Do; McCormick, Donald B.
 CORPORATE SOURCE: Sch. Med., Emory Univ., Atlanta, GA, 30322, USA
 SOURCE: Arch. Biochem. Biophys. (1980), 204(1), 41-51
 CODEN: ABBIA4; ISSN: 0003-9861
 DOCUMENT TYPE: Journal
 LANGUAGE: English

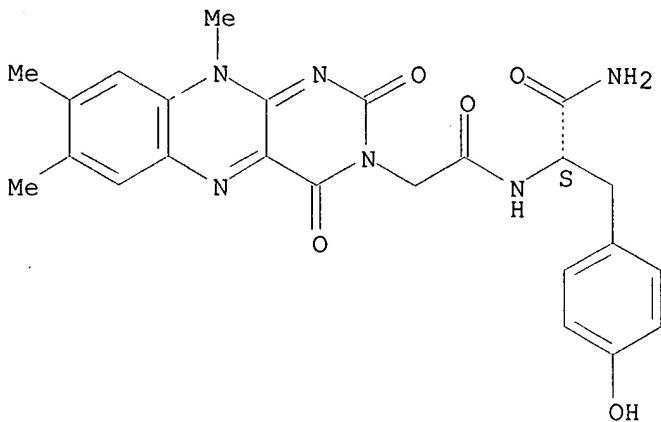
AB The properties of the riboflavin-binding site in the riboflavin-binding protein from egg white have been elucidated by detg. consts. for binding of flavin analogs to the protein and by changes in absorption spectra of free and bound flavins. The spectral changes and unfavorable interaction of the protein with charged species indicate that the overall flavin environment in the holoprotein is hydrophobic. Modification of either ring or side-chain portions of flavin usually results in a decrease of binding energy. Although no one portion of the structure is absolutely essential, both 7- and 8-Me groups and 2'-OH group contribute most significantly to binding. The binding site at the region of C-2 and N-3 of the isoalloxazine is rather insensitive to the relative site of a substituent and thus relatively open, whereas considerable steric limitation is imposed at C-8, N-10, esp. C-1', and 4-carbonyl positions. The OH groups of the N-10 side chain contribute in a stereoselective manner by formation of H bonds. Studies with model compds. that represent only a part of flavin suggest that the dimethylbenzenoid portion of the ring is involved in primary interactions of binding, and relatively buried in the protein. The quenching of protein fluorescence on binding is mainly due to ground-state stacking interaction between a tryptophanyl residue at the binding site and the quinoxaline portion, and not to Foerster energy transfer.

IT 75560-19-9

RL: PRP (Properties)
 (assocn. of, with riboflavin-binding protein)

RN 75560-19-9 CAPLUS
 CN Benzenepropanamide, .alpha.-[[[4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl]acetyl]amino]-4-hydroxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 44 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:127954 CAPLUS

DOCUMENT NUMBER: 92:127954

TITLE: Molecular luminescence of some isoalloxazines in apolar solvents at various temperatures

AUTHOR(S): Eweg, Jan K.; Mueller, Franz; Visser, Antonie J. W.
G.; Veeger, Cees; Bebelaar, Dick; Von Voorst, Joop D.
W.

CORPORATE SOURCE: Dep. Biochem., Agric. Univ., Wageningen, 6703 BC,
Neth.

SOURCE: Photochem. Photobiol. (1979), 30(4), 463-71

CODEN: PHCBAP; ISSN: 0031-8655

DOCUMENT TYPE: Journal

LANGUAGE: English

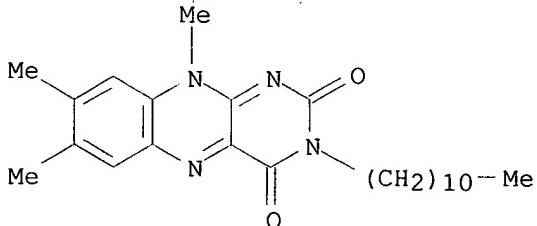
AB The electronic spectral properties of isoalloxazines in org. solvents of low polarity were detd. at 300 and 77 K. Vibrational structure in the spectra show a vibrational mode at 1250 cm⁻¹. The pure electronic transition energies were detd. accurately and compared with theor. data. Actual lifetimes are up to 10 ns for fluorescence and 300 ms for phosphorescence. The ratio of the actual fluorescence lifetime and the radiative lifetime agrees with the quantum field. Solvent interactions hardly shift the energy of the first electronically excited singlet state but merely affect the Franck-Condon envelope of the spectrum and the nonradiative decay of the chromophore. In alkane solns. at 77 K isoalloxazine clusters are formed showing P-type delayed fluorescence.

IT 73057-72-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and absorption and luminescence spectra of)

RN 73057-72-4 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-undecyl- (9CI)
(CA INDEX NAME)



L37 ANSWER 45 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1979:606691 CAPLUS
 DOCUMENT NUMBER: 91:206691
 TITLE: The measurement of subnanosecond fluorescence decay of flavins using time-correlated photon counting and a mode-locked argon ion laser
 AUTHOR(S): Visser, A. J. W. G.; Van Hoek, A.
 CORPORATE SOURCE: Dep. Biochem., Agric. Univ., Wageningen, 6703 BC, Neth.
 SOURCE: J. Biochem. Biophys. Methods (1979), 1(4), 195-208
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A system is described consisting of a mode-locked Ar ion laser and time-resolved photon-counting electronics. The system can measure fluorescence lifetimes in the subnanosecond time domain. The Ar ion laser is suitable for the excitation of flavins since the available laser wavelengths encompass the 1st absorption band of the yellow chromophore. Due to the high radiation d. and the short pulse, both the time and wavelength resoln. of the fluorescence of very weakly emitting compds. can be measured. Expts. are described for flavin models exhibiting single and multiple modes of decay. In these examples, lifetimes were detd. both from deconvolved decay curves and from direct anal. of the tail of the curve, where no interference of the exciting pulse is encountered. Both detns. showed very good agreement. Due to the highly polarized laser light, the decay of the emission anisotropy could be measured directly after the exciting pulse. In principle, fast rotational motions might be detected. An anisotropy measurement conducted with a flavoprotein with a noncovalently attached FAD is presented.

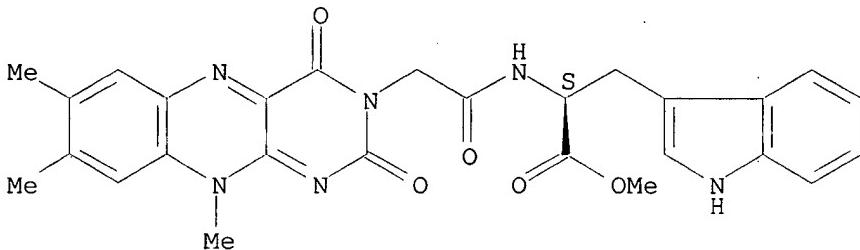
IT 21099-87-6

RL: ANST (Analytical study)
(fluorescence decay of, detn. with argon laser)

RN 21099-87-6 CAPLUS

CN L-Tryptophan, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 46 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1980:17253 CAPLUS
 DOCUMENT NUMBER: 92:17253
 TITLE: Flavin-dependent substrate photooxidation as a chemical model of dehydrogenase action
 AUTHOR(S): Haas, Wolfgang; Hemmerich, Peter
 CORPORATE SOURCE: Dep. Biol., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
 SOURCE: Biochem. J. (1979), 181(1), 95-105
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB As a model of flavin-dependent biol. dehydrogenation, flavin-sensitized

photodehydrogenation and photodecarboxylation were studied by variation of substrate, flavin, pH, and solvent. The following rules were then derived. When the reactive site of a photosubstrate is an .alpha.-C atom of the type :CH-CO₂-, decarboxylation is preferred to dehydrogenation, whereas the reverse is true for the neutral :CH-CO₂H. Consequently, these reactions do not exhibit a measurable isotope effect with :C₂H-CO₂-, in contrast with the findings of G. P. Penzer et al. (1970), which could not be reproduced. When the substrate does not contain a carboxylate group, isotope effects occur. The mechanism of flavin-sensitized substrate photodecarboxylation is assumed to consist of a primary carbanion fixation at the flavin nucleus (position 4a, 5, or 8) with concomitant liberation of CO₂. This step is followed by rapid fragmentation of the adduct :CH-F1-red., provided that the substrate contained a functional and electron-donating group, e.g. X = OH, OMe, or NH₂ (but not NH₃⁺) in -CHX-CO₂-.

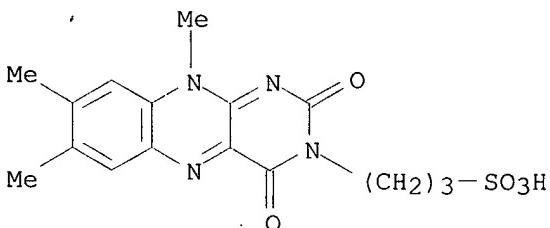
The min. requirement for flavin-sensitized C-H dehydrogenation is the presence of an OH group. E.g., MeOH as substrate and solvent is dehydrogenated at pH sufficiently alk. for detection of the presence of the active species MeO⁻, whereas at more acidic pH, substrate dehydrogenation is competing with flavin autoprotolysis, which depends on the substituents in the flavin nucleus.

IT 36469-13-3

RL: BIOL (Biological study)
(photooxidn. dependent on)

RN 36469-13-3 CAPLUS

CN Benzo[g]pteridine-3(2H)-propanesulfonic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



L37 ANSWER 47 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1979:485819 CAPLUS

DOCUMENT NUMBER: 91:85819

TITLE: On the environment and the rotational motion of amphiphilic flavins in artificial membrane vesicles as studied by fluorescence

AUTHOR(S): Schmidt, Werner

CORPORATE SOURCE: Dep. Biol., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.

SOURCE: J. Membr. Biol. (1979), 47(1), 1-25
CODEN: JMBBBO; ISSN: 0022-2631

DOCUMENT TYPE: Journal

LANGUAGE: English

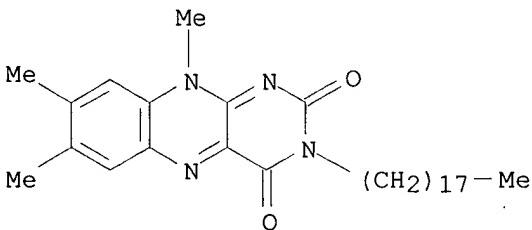
AB The incorporation of 4 amphiphilic flavins (amphiflavins) as fluorescence markers bearing C₁₈-hydrocarbon chains at various positions of the chromophore into artificial membrane vesicles was investigated. The vesicles utilized were made from 3 different satd. phospholipids. The stability of the flavin-charged vesicles was good over several days, depending somewhat on the temp., the pH, and their concn. A marked increase of the fluorescence quantum yield near the vesicle phase transition (cryst. .fwdarw. liq.-cryst.) was found which indicated that the flavin nuclei are imbedded more deeply into the hydrophobic portion of the membranes. This is further supported by a hypsochromic shift of the flavin near-UV peak and the increase of absorbance at 450 nm upon melting.

Rotational relaxation times of the various amphiflavins bound to the different vesicles were obtained from measurements of the fluorescence polarizations as a function of temp. From these data, the microviscosities in the region of the chromophores were calcd. Measurements of the fluorescence polarization as a function of the solvent viscosity and vesicle phase (cryst.-liq.-cryst.) indicated that below the phase transition the flavin nucleus is protected from the suspension medium by a lipid-water interphase, which softens above the phase transition. The dependence of the flavin orientation and microenvironment on the position of the substitution of the aliph. chain is reflected in the differences of the fluorescence yields and the shape of the emission spectra.

IT 53965-14-3

RL: BIOL (Biological study)
(liposome-bound, fluorescence of, environment and rotational motion of)

RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
(CA INDEX NAME)

L37 ANSWER 48 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1978:575315 CAPLUS
DOCUMENT NUMBER: 89:175315
TITLE: Photoejection of electrons from flavins in polar media
AUTHOR(S): Getoff, N.; Solar, S.; McCormick, D. B.
CORPORATE SOURCE: Inst. Theor. Chem. Strahlenchem., Univ. Wien, Vienna,
Austria
SOURCE: Science (1978), 201(4356), 616-18
CODEN: SCIEAS; ISSN: 0036-8075

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Riboflavin and 12 of its derivs.s formed solvated electrons under UV irradn. (253.7 nm) in various H₂O-MeOH solvent mixts. The highest quantum yield of solvated electrons (.apprx.0.03) was obtained for flavins contg. tyrosine on a side chain in the isoalloxazine N-3 or N-10 position. The splitting of H atoms from excited flavin mols. was also obsd. It was detd. that the semiquinone transients are formed not only by way of the flavin triplet, as usually suggested, but also by the attack of the electrons and H atoms on flavin mols. in the ground state. This is important, because the flavin radicals remaining after the electron-ejection or H-splitting processes must also be considered in the subsequent reaction mechanisms. The electron-ejection process from electronically excited flavins has important implications in the photobiol. of these compds.

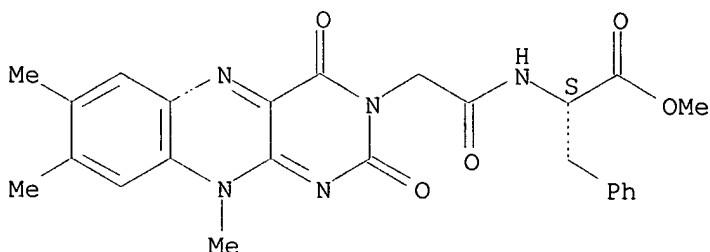
IT 20507-92-0 20806-70-6 21099-87-6

RL: PRP (Properties)
(polaron ejection from excited state of, after UV radiation)

RN 20507-92-0 CAPLUS

CN L-Phenylalanine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

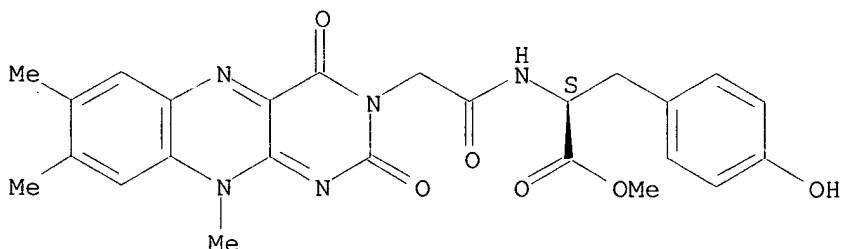
Absolute stereochemistry.



RN 20806-70-6 CAPLUS

CN L-Tyrosine, N-[{(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl}]-, methyl ester (9CI) (CA INDEX NAME)

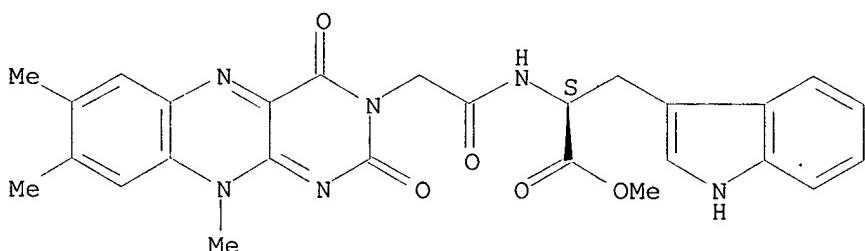
Absolute stereochemistry.



RN 21099-87-6 CAPLUS

CN L-Tryptophan, N-[{(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl}]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 49 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1978:444179 CAPLUS

DOCUMENT NUMBER: 89:44179

TITLE: Synthesis of some ethyl esters of N-(8-riboflavinoyl)amino acids

AUTHOR(S): Sluke, J.; Grinsteins, V.

CORPORATE SOURCE: Latv. Gos. Univ., Riga, USSR

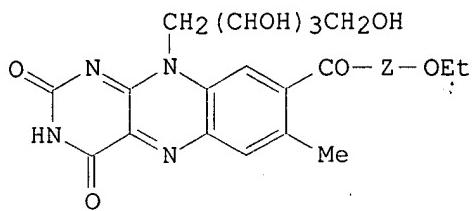
SOURCE: Latv. PSR Zinat. Akad. Vestis, Kim. Ser. (1978), (2), 241

CODEN: LZAKAM; ISSN: 0002-3248

DOCUMENT TYPE: Journal

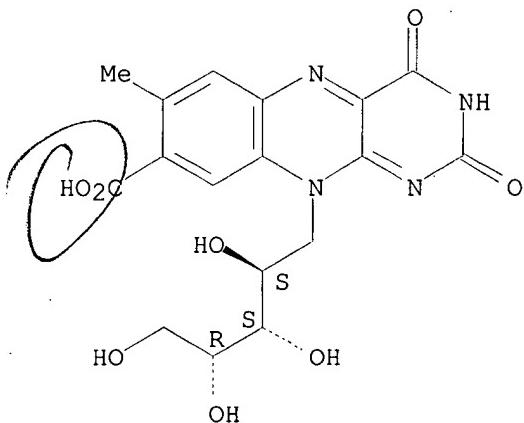
LANGUAGE: Russian

GI

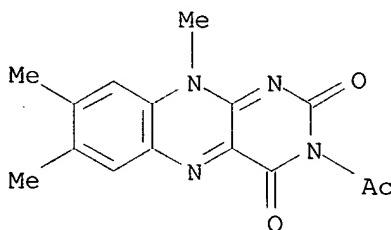


AB Condensation of 8-carboxy-8-demethylriboflavine with H-Gly-OEt and H-Val-OEt in the presence of dicyclohexylcarbodiimide gave 21-5% I (Z = Gly, Val).
 IT **28083-73-0**
 RL: RCT (Reactant)
 (condensation of, with amino acid)
 RN 28083-73-0 CAPLUS
 CN Riboflavin, 8-carboxy-8-demethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 50 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1978:85395 CAPLUS
 DOCUMENT NUMBER: 88:85395
 TITLE: A versatile apparatus for performing anaerobic optical titrations with provision for multiple sampling of the reaction mixture
 AUTHOR(S): Palmer, Graham
 CORPORATE SOURCE: Dep. Biochem., Rice Univ., Houston, Tex., USA
 SOURCE: Anal. Biochem. (1977), 83(2), 597-608
 CODEN: ANBCA2; ISSN: 0003-2697
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB An all-glass device suitable for the oxidoreductive titrn. of air-sensitive compds. is described. The device has a provision for monitoring the optical spectrum and for sampling the reaction mixt. with direct transfers of the sample into EPR sample tubes. The performance of the device is evaluated and an example of its use is given.
 IT **60823-53-2**
 RL: PROC (Process)
 (titrn. of, app. for)
 RN 60823-53-2 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-acetyl-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 51 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:573100 CAPLUS

DOCUMENT NUMBER: 85:173100

TITLE: Spectral properties of fluorescent dyes in lecithin vesicles. Probes for the structure of lipid bilayer membranes and for membrane potentials

AUTHOR(S): Pohl, G. W.

CORPORATE SOURCE: Fachber. Biol., Univ. Konstanz, Constance, Ger.

SOURCE: Z. Naturforsch., C: Biosci. (1976), 31C(9-10), 575-88

CODEN: ZNCBDA

DOCUMENT TYPE: Journal

LANGUAGE: English

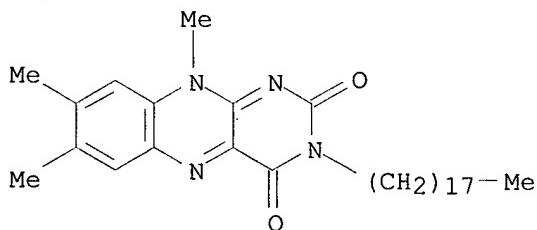
AB Three fluorescent dyes (a merocyanine, a cyanine, and a modified umbelliferone) were incorporated into vesicles from 3 different lecithins. Their absorption spectrum, emission spectrum, and fluorescence polarization in the lipid vesicles were studied and compared with the spectral properties in homogeneous org. solns. The reactivity of lipid-bound dyes with reagents in the aq. phase was investigated. The location of various dyes in the lipid membrane and their use as indicators of phase transitions or membrane potentials are discussed.

IT 53965-14-3

RL: PRP (Properties)
(fluorescent polarization of, in lecithin bilayer membranes)

RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
(CA INDEX NAME)



L37 ANSWER 52 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:577838 CAPLUS

DOCUMENT NUMBER: 85:177838

TITLE: Synthesis, separation, identification and interconversion of riboflavin phosphates and their acetyl derivatives: a reinvestigation

AUTHOR(S): Scola-Nagelschneider, Gisela; Hemmerich, Peter

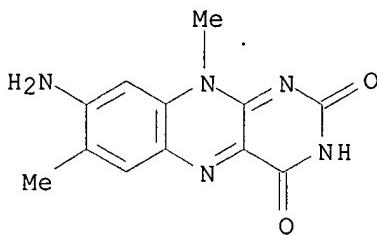
CORPORATE SOURCE: Fachber. Biol., Univ. Konstanz, Konstanz, Ger.

SOURCE: Eur. J. Biochem. (1976), 66(3), 567-77

CODEN: EJBCAI

DOCUMENT TYPE: Journal

LANGUAGE: English



L37 ANSWER 61 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1972:448772 CAPLUS

DOCUMENT NUMBER: 77:48772

TITLE: Synthesis and properties of 8. α -substituted riboflavines of biological importance

AUTHOR(S): Kenney, William C.; Walker, Wolfram H.

CORPORATE SOURCE: Mol. Biol. Div., Veterans Adm. Hosp., San Francisco, Calif., USA

SOURCE: FEBS (Fed. Eur. Biochem. Soc.) Lett. (1972), 20(3), 297-301

CODEN: FEBLAS

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB 8. α -Substituted riboflavines (I, II, III, and IV) were prep'd. Thus, 8. α -bromotetraacetylriboflavine (V) was reacted with . α -(N-benzoyl)-L-lysine acetate in DMF to give a product which on hydrolysis gave 8. α -(N. ϵ -lysyl)riboflavine (I). Similarly prep'd. were 8. α -(O-tyrosyl)riboflavine (II) and 8. α -sulforiboflavine (III). The carboxylic acid (IV) was obtained from V by performic acid oxidn. Properties of I, II, III, and IV are compared with those of some other 8. α -substituted riboflavines.

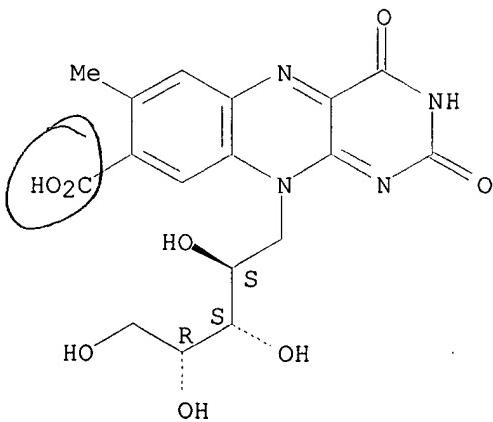
IT 28083-73-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 28083-73-0 CAPLUS

CN Riboflavin, 8-carboxy-8-demethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

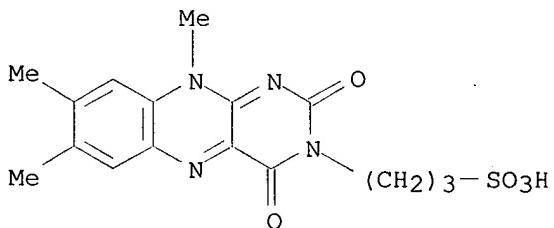


L37 ANSWER 62 OF 72 CAPLUS COPYRIGHT 2002 ACS

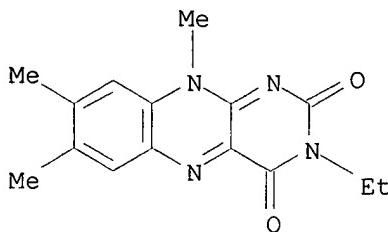
ACCESSION NUMBER: 1972:96079 CAPLUS

DOCUMENT NUMBER: 76:96079

TITLE: Flavine cations. Ground and excited states properties
 AUTHOR(S): Lhoste, J. M.
 CORPORATE SOURCE: Sect. Biol., Fond. Curie-Inst. Rad., Paris, Fr.
 SOURCE: Eur. Biophys. Congr., Proc., 1st (1971), Volume 4,
 221-5. Editor(s): Broda, E. Verlag Wiener Med.
 Akad.: Vienna, Austria.
 CODEN: 24KMAA
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB Fluorescence of the neutral and cationic forms of the flavines were studied using low-temp. (-196.degree.) glasses or polyvinyl alc.-stretched films. The cationic flavines had about the same quantum efficiency as neutral flavines in the solid state.
 IT 36469-13-3
 RL: RCT (Reactant)
 (spectral properties of)
 RN 36469-13-3 CAPLUS
 CN Benzo[g]pteridine-3(2H)-propanesulfonic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



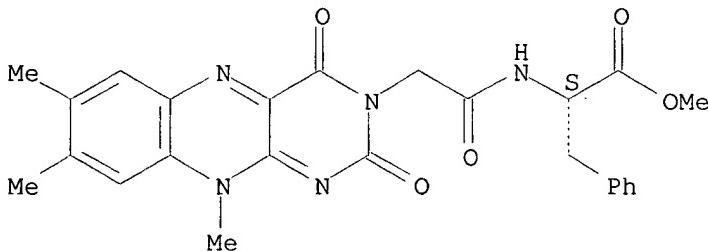
L37 ANSWER 63 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1970:431535 CAPLUS
 DOCUMENT NUMBER: 73:31535
 TITLE: Kinetics and mechanism of oxidation-reduction reactions between pyridine nucleotides and flavins
 AUTHOR(S): Wu, Felicia Y. H.; MacKenzie, Robert E.; McCormick, Donald B.
 CORPORATE SOURCE: Div. of Biol. Sci., Cornell Univ., Ithaca, N. Y., USA
 SOURCE: Biochemistry (1970), 9(11), 2219-24
 CODEN: BICHAW
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The oxidn. of reduced pyridine nucleotides or analogs by equimolar flavine or flavinyl peptide was measured to det. the influences of mol. interactions between the amino acid residue and flavine prosthetic group and between the latter and the pyridine nucleotide. For peptides with substitution at position N-10 of the flavine, the rates follow alanyl > phenylalanyl > tyrosyl > tryptophanyl. This order varies inversely with the degree of intramol. complexing between the given amino acid and the flavine portion. Increased temp. slightly increases the rates. Generally similar results were obsd. for the N-3 series as with N-10 flavines. Overall, the results confirm a H- mechanism with initial addn. at the flavine N-5.
 IT 20469-92-5 20507-92-0 20806-70-6
 21099-87-6
 RL: RCT (Reactant)
 (reaction of, with reduced pyridine nucleotides, kinetics of)
 RN 20469-92-5 CAPLUS
 CN Lumazine, 3-ethyl- (8CI) (CA INDEX NAME)



RN 20507-92-0 CAPLUS

CN L-Phenylalanine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

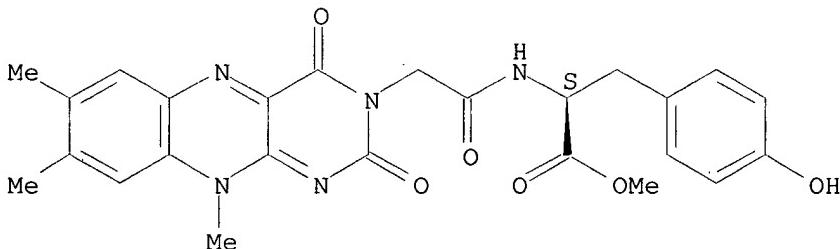
Absolute stereochemistry.



RN 20806-70-6 CAPLUS

CN L-Tyrosine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

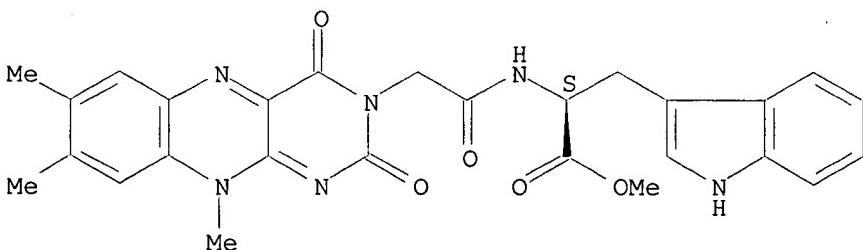
Absolute stereochemistry.



RN 21099-87-6 CAPLUS

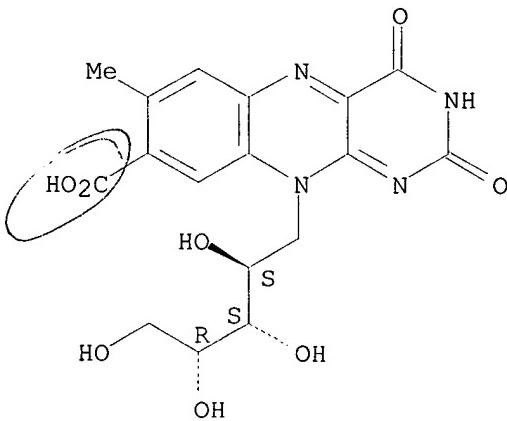
CN L-Tryptophan, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 64 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1970:121860 CAPLUS
 DOCUMENT NUMBER: 72:121860
 TITLE: Flavine derivatives via bromination of the 8-methyl substituent
 AUTHOR(S): McCormick, Donald B.
 CORPORATE SOURCE: Grad. Sch. of Nutr., Cornell Univ., Ithaca, N. Y., USA
 SOURCE: J. Heterocycl. Chem. (1970), 7(2), 447-50
 CODEN: JHTCAD
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Acetylation of riboflavin with Ac₂O gave a tetraacetyl deriv., which treated with Br and pyridine gave a complex of brominated tetraacetylriboflavin with dibromopyridine. The complex treated with aq. acid gave 2',3',4',5'-tetraacetyl-8,.omega.-dibromoriboflavin, which was hydrolyzed to 8-formyl-riboflavin (I). I condensed with 2,4-dinitrophenylhydrazine gave 8-formylriboflavin 2,4-dinitrophenylhydrazone. Peracetylation of I gave 2',3',4',5'-tetraacetyl-8-formylriboflavin. Oxidn. of I gave 8-carboxyriboflavin. I was phosphorylated at the 5'-hydroxymethyl function to give 8-formylriboflavin 5'-phosphate, which was condensed with adenosine 5'-phosphoromopholidate to yield 8-formylriboflavin-adenine dinucleotide.
 IT 28083-73-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 28083-73-0 CAPLUS
 CN Riboflavin, 8-carboxy-8-demethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 65 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1969:409625 CAPLUS
 DOCUMENT NUMBER: 71:9625
 TITLE: Flavanyl peptides. II. Intramolecular interactions in flavanyl aromatic amino acid peptides
 AUTHOR(S): MacKenzie, Robert E.; Foery, Werner; McCormick, Donald B.
 CORPORATE SOURCE: Cornell Univ., Ithaca, N. Y., USA
 SOURCE: Biochemistry (1969), 8(5), 1839-44
 CODEN: BICHAW
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Close assocn. of flavine coenzymes with aromatic amino acid residues as may occur in flavoproteins was simulated with a model system. L-Tryptophan, L-tyrosine, and L-phenylalanine were attached by peptide

linkage to N-3 and N-10 .omega.-carboxyalkylflavines. The dependence of spectral and fluorescence properties of the flavine upon variation of the chain length sepg. the two chromophores was investigated. Fluorescence quenching due to collisions in the excited state, but esp. that due to ground-state complex formation, increases as the chain length of the 10-substituted flavinyltryptophan and -tyrosine peptides decreases from 5 to 1 methylene groups. Hydrophobic forces are undoubtedly involved in complex formation in aq. soln., but dispersion forces are also effective, since significant fluorescence quenching occurs in org. solvents. The flavinyltyrosine peptides exhibit intramol. H bonding between the tyrosine OH and the 4-carbonyl group of the flavine in CHCl₃, but this is not the most important force in maintaining interaction in aq. soln.

Flavinyltryptophan and -tyrosine peptides (n = 1) in position 10 of the flavine have fluorescence properties which differ from those of the corresponding peptides substituted in position 3. This indicates that orientation of the complexing moieties influences the extent and type of quenching of the flavine fluorescence. Short-chain flavinyl peptides exhibit a degree of fluorescence quenching of sufficient magnitude to account for similar changes observed upon binding of flavinyl coenzymes to apoenzymes.

IT 20806-70-6 21099-87-6

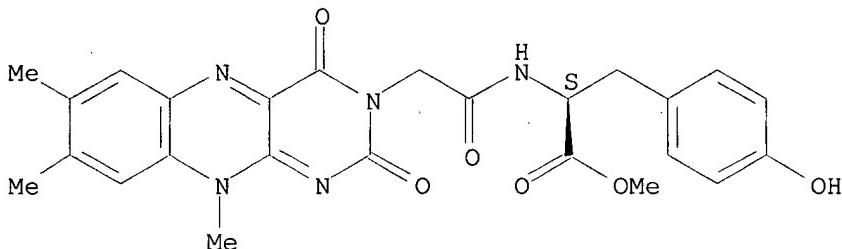
RL: BIOL (Biological study)

(fluorescent quenching of, intramol. interactions in)

RN 20806-70-6 CAPLUS

CN L-Tyrosine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

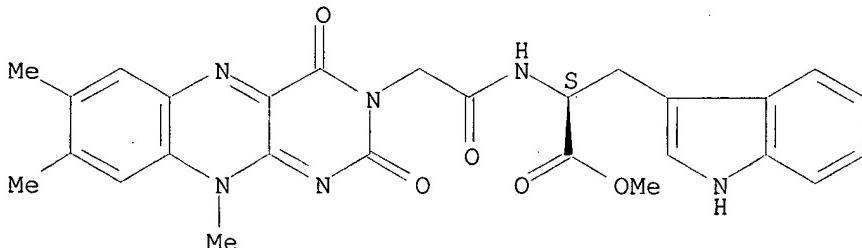
Absolute stereochemistry.



RN 21099-87-6 CAPLUS

CN L-Tryptophan, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 66 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:7791 CAPLUS

DOCUMENT NUMBER: 72:7791

TITLE: Optical and electron spin resonance spectra of flavine neutral and cation radicals in nonpolar solvents

AUTHOR(S): Walker, Wolfram H.; Ehrenberg, Anders
 CORPORATE SOURCE: Stockholms Univ., Stockholm, Swed.
 SOURCE: FEBS (Fed. Eur. Biochem. Soc.) Lett. (1969), 3(5),
 315-18
 CODEN: FEBLAL
 DOCUMENT TYPE: Journal
 LANGUAGE: English

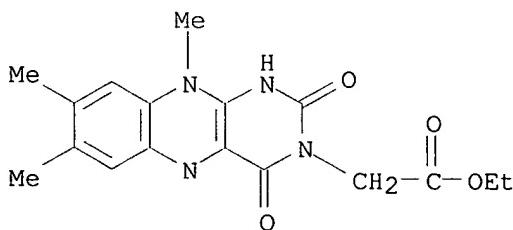
AB The following lumiflavine derivs. were prepared: 3-(ethoxycarbonylmethyl)lumiflavine (I); 3-methyl-5-benzyl-1,5-dihydrolumiflavine (II), and 3-methyl-4a-hydroxy-5-benzyl-4a,5-dihydrolumiflavine (III). The green-colored neutral radical was produced by dissolving anaerobically equiv. amts. of II and III in the appropriate solvent (C6H6 or PhMe). The 5-methyl or 5-deuteriomethyl substituted flavine radical was obtained by reductive alkylation of I with CH3I or CD3I. By the addn. of CF3CO2H to the neutral radical solns., the cations are formed. The 5-unsubstituted cation radical was prep'd. by anaerobic redn. of I with solid Na2S2O4 in C6H6 + CF3CO2H/CF3CO2D. The absorption spectrum of 5-benzylated lumiflavine cation and that of neutral radical showed that the solvent affects the spectrum of the neutral radical drastically. This radical is blue in water and green in C6H6. The long-wavelength doublet band at 675 and 623 nm in pure C6H6 shifts to shorter wavelength and collapses under extinction lowering with higher solvent polarity. The 3,5-disubstituted cation radical in C6H6 showed 2 pronounced absorption bands at 505 and 352 nm. Anaerobic redn. of the pale yellow cation with solid dithionite resulted in isosbestic points at 362 and 444 nm. The redn. stopped when the extinction at 493 nm reached its max. The absorption at 395 nm reached a min. at the same time. Redn. of flavine with Zn did not result in isosbestic points. ESR recordings were made at room temp. and a radical concn. of 0.5 mM o f the 3- and 5-substituted lumiflavine neutral radicals in C6H6 and of the cation radicals in C6H6 + 10% CF3CO2H. The coupling const. of the .alpha.-proton attached to N-5 for the cation radical is 11.5 gauss. That of the .beta.-protons of the 5-N-methyl group for the neutral radical is 8.5 gauss. Comparison of the ESR spectra of the 2 cations indicated that only one methylene proton of the 5-benzyl group is strongly coupling. By using PhMe as solvent, the temp. effect on the hyperfine structure (hfs) of the neutral radicals was studied at -120.degree.-60.degree.. Freezing of the solvent at -95.degree. abolished the hfs for both radicals. At .apprx.-10.degree., there is a temp. optimum for the hfs resoln. The change of hfs resoln. was a result of a change of the mobility of the methylene protons.

IT 25767-03-7 27901-98-0

RL: PRP (Properties)
 (electron spin resonance spectrum of)

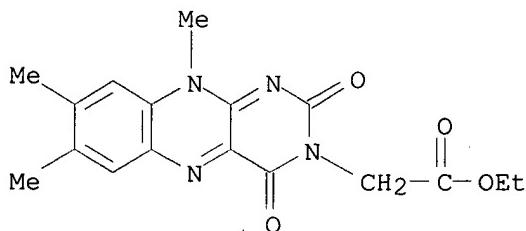
RN 25767-03-7 CAPLUS

CN Benzo[g]pteridinium-5-yl, 3-(carboxymethyl)-1,2,3,4,5,10-hexahydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (8CI) (CA INDEX NAME)



H+

RN 27901-98-0 CAPLUS
 CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester, conjugate monoacid (8CI) (CA INDEX NAME)

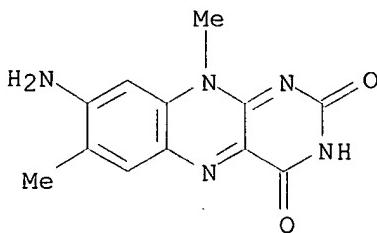


● H⁺

L37 ANSWER 67 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1969:56978 CAPLUS
 DOCUMENT NUMBER: 70:56978
 TITLE: Allo- and isoalloxazine. XXI. Ir spectra and tautomers of alloxazines
 AUTHOR(S): Berezovskii, V. M.; Aksel'rod, Zh. I.; Fetisova, T. P.; Kustanovich, I. M.; Polyakova, N. A.
 CORPORATE SOURCE: Vses. Nauch.-Issled. Vitamin. Inst., Moscow, USSR
 SOURCE: Zh. Obshch. Khim. (1968), 38(11), 2449-57
 CODEN: ZOKHA4
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian

AB The previously reported alloxazines were examd. as to their ir spectra. Alloxazine and isoalloxazine structures can be distinguished through differences in absorption in the 1700-cm.⁻¹ and 1600-1500-cm.⁻¹ regions. In the cryst. state and in aprotic solvents the alloxazines with unfixed structure exist mainly as alloxazines proper. Among 7-amino derivs. the differences in ir spectra of the 2 families become smaller but it is still possible to assign the largely alloxazine structure to most of the unfixed aminoalloxazines and 1,3-dimethyl-7-aminoalloxazine; these show some double bond character in their C-N1 bond. The 7-aminoalloxazines exist specifically as the amino derivs. rather than as imino forms. In the anions of alloxazines, regardless of the nature of the co-cation present, the electron d. approaches that found in lactim compds. The ir spectra of 36 compds. are reported.

IT 3942-96-9
 RL: PRP (Properties)
 (spectrum of, ir)
 RN 3942-96-9 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 68 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:451281 CAPLUS

DOCUMENT NUMBER: 69:51281

TITLE: Base-catalyzed hydrolysis of flavines. Effect of amines and the particular role of Position 3

AUTHOR(S): McCormick, Donald B.; Foery, Werner

CORPORATE SOURCE: Cornell Univ., Ithaca, N. Y., USA

SOURCE: J. Pharm. Sci. (1968), 57(5), 841-4

CODEN: JPMSAE

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The base-catalyzed hydrolysis of flavines was investigated in 50% water-MeOH with excess NaOH or excess amines at different temps. Rate consts. for the pseudo first-order cleavage of the pyrimidine portion of the isoalloxazine systems were measured and with NaOH shown to increase from lumiflavine to 3-ethylumiflavine to 3-carboxyamido(phenylalanyl)lumi flavine. With amines, the size as well as basicity is of prime importance since the general order in efficacy of the nucleophile for hydrolysis of flavines is EtNH₂ > Et₂NH > Et₃N > PhCH₂NH₂ > Bu₃N. In general, alkylation of the 3-imino function of the flavine increases its lability because of inability to ionize and undergo resonance stabilization of the anionic tautomers. Moreover, the special case where a 3-carboxamido function is present allows intramol. polarization, via H bonding of the amide H to 4-carbonyl O which causes a marked increase in hydrolysis rate in NaOH. From the temp. dependencies of the rates of hydrolysis, the calcd. values for energies of activation indicate a decrease expected upon 3-alkylation and further upon intramol. enhancement with the 3-carboxamido group. The calcd. values for entropies of activation are large and neg. in accord with considerable loss of degrees of freedom in the activated complexes formed in the bimol. mechanism.

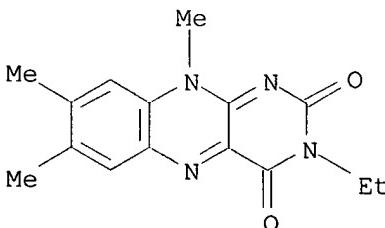
IT 20469-92-5 20507-92-0

RL: RCT (Reactant)

(hydrolysis of, in presence of amines, kinetics of)

RN 20469-92-5 CAPLUS

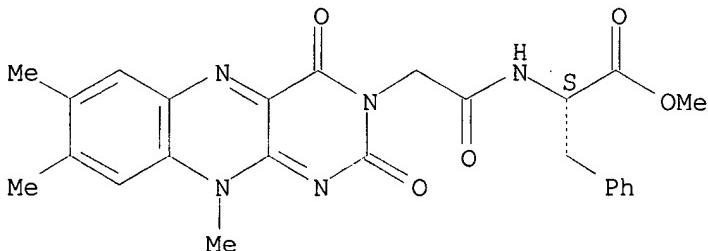
CN Lumazine, 3-ethyl- (8CI) (CA INDEX NAME)



RN 20507-92-0 CAPLUS

CN L-Phenylalanine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 69 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1969:4566 CAPLUS

DOCUMENT NUMBER: 70:4566

TITLE: Flavvinyl peptides. I. Synthesis of flavinyl-aromatic amino acids

AUTHOR(S): Foery, Werner; MacKenzie, Robert E.; McCormick, Donald B.

CORPORATE SOURCE: Cornell Univ., Ithaca, N. Y., USA

SOURCE: J. Heterocycl. Chem. (1968), 5(5), 625-30

CODEN: JHTCAD

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The syntheses of flavinyl peptides, in which L-tryptophan, L-tyrosine, or L-phenylalanine are attached via peptide linkage to the isoalloxazine system with .omega.-carboxyalkyl groups in position 3 or 10, are described. Lumiflavin was carboxymethylated by known methods to yield N-3-carboxymethylllumiflavin. Oxidn. of 10-.omega.-hydroxyhexyl-, 10-.omega.-hydroxypentyl-, 10-.omega.-hydroxybutyl-, and 10-formylmethylflavins gave the corresponding 10-.omega.-carboxyalkylflavins (I) (n = 3, etc.). The 10-.omega.-carboxyethylflavin was obtained by condensation of 2-amino-4,5-dimethyl-N-.omega.-carboxyethylalanine with alloxan. Activations of the carboxyl group of the flavins were achieved with N,N'-carbonyldimidazole and p-nitrophenyltri-fluoroacetate to form the corresponding acylimidazoles and p-nitrophenyl esters. 10-Carboxymethylhydroflavin was hydrogenated to form 10-carboxymethylhydroflavin and activated by carbodiimide. Reaction of the carboxy-activated flavins with the appropriate amino acid methyl esters, followed by air oxidn. in the case of dihydroflavin, gave the corresponding flavinyl peptides. Interaction of the flavin with aromatic amino acids results in a broadening of the visible flavin absorption towards the green, without the appearance of discrete new max., and in quenching of the flavin fluorescence. The fluorescence efficiency increases with increasing numbers of methylene groups in the flavin side chain. The nonlinear dependency of fluorescence quenching versus no. of methylene groups indicates that different types of intramol. interactions are involved.

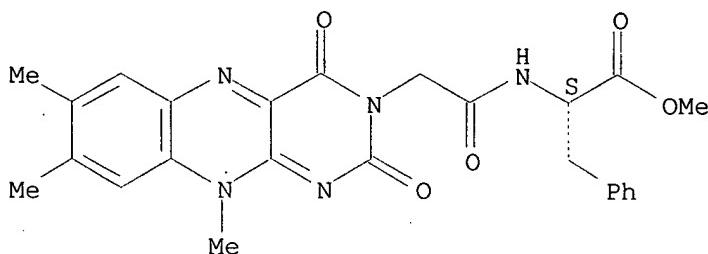
IT 20507-92-0P 20806-70-6P 21099-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 20507-92-0 CAPLUS

CN L-Phenylalanine, N-[{(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl}], methyl ester (9CI) (CA INDEX NAME)

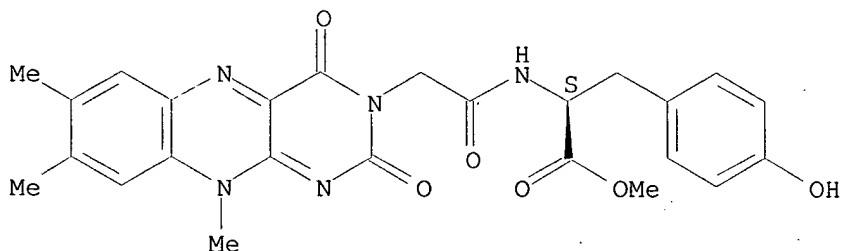
Absolute stereochemistry.



RN 20806-70-6 CAPLUS

CN L-Tyrosine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

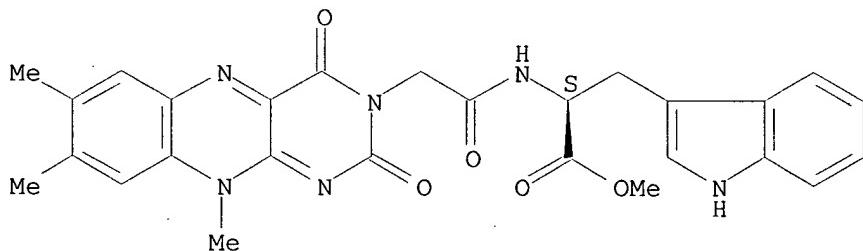
Absolute stereochemistry.



RN 21099-87-6 CAPLUS

CN L-Tryptophan, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L37 ANSWER 70 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:118395 CAPLUS

DOCUMENT NUMBER: 68:118395

TITLE: Basicity, visible spectra, and electron spin resonance
of flavosemiquinone anions

AUTHOR(S): Ehrenberg, Anders; Mueller, Franz; Hemmerich, Peter

CORPORATE SOURCE: Med. Nobelinstit., Karolinska Inst., Stockholm, Swed.

SOURCE: Eur. J. Biochem. (1967), 2(3), 286-93

CODEN: EJBCAI

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The dependence on pH of the disproportionation of the flavosemiquinone was
investigated by E.S.R. For 3-(R-substituted)-lumiflavine (R = CH₂COO⁻) in
aq. soln. pK_a (for the dissoctn. of the neutral flavosemiquinone) is 8.4;
pK_{red} is 6.3. Hydrolytic ring cleavage in position 2, 8.8'-dimerization,
and 10-dealkylation interfere with the formation of the flavosemiquinone

anion. However, in nonaq. HCONMe₂ and with stoichiometric amts. of strong base (tert-BuOK), 100% flavosemiquinone anion is formed without interfering side reactions. Its light absorption spectrum is practically identical to that of the "red flavoprotein radical." From the E.S.R. spectra the individual isotropic hyperfine coupling consts. were detd. 27 references.

IT 20409-01-2

RL: PRP (Properties)
(electron spin resonance and visible spectrum of)

RN 20409-01-2 CAPLUS

L37 ANSWER 71 OF 72 USPATFULL

ACCESSION NUMBER: 2001:165571 USPATFULL

TITLE: Isoalloxazine derivatives to neutralize biological
contaminantsINVENTOR(S): Platz, Matthew Stewart, Columbus, OH, United States
Goodrich, Raymond Paul, JR., Denver, CO, United States

NUMBER KIND DATE

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PATENT INFORMATION: US 2001024781 A1 20010927

APPLICATION INFO.: US 2001-777727 A1 20010205 (9)

RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 1999-420652, filed
on 19 Oct 1999, GRANTED, Pat. No. US 6268120

DOCUMENT TYPE: Utility

FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: Greenlee, Winner and Sullivan, P.C., Suite 201, 5370
Manhattan Circle, Boulder, CO, 80303

NUMBER OF CLAIMS: 63

EXEMPLARY CLAIM: 1

LINE COUNT: 1453

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Methods are provided for neutralization of microorganisms in fluids or on surfaces. Preferably the fluids contain blood or blood products and comprise biologically active proteins. Preferred methods include the steps of adding an activation-effective amount of a microorganism neutralizer with an isoalloxazine backbone to a fluid and exposing the fluid to a triggering event. Preferred triggering events include light of a suitable wavelength and intensity to activate the microorganism neutralizer or a pH sufficient to activate the microorganism neutralizer. Other fluids, including juices, water and the like, may also be decontaminated by these methods as may surfaces of foods, animal carcasses, wounds, food preparation surfaces and bathing and washing vessel surfaces. Compounds with an isoalloxazine backbone are also provided.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

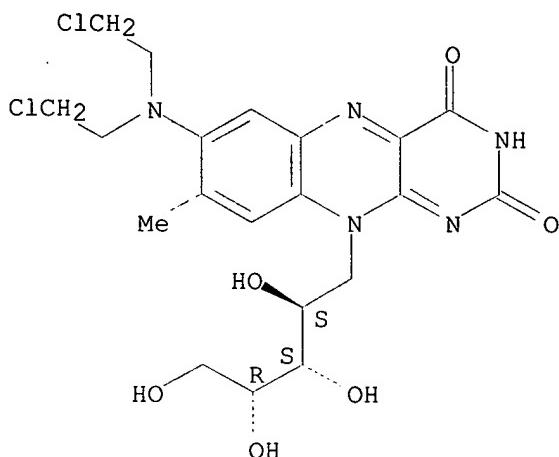
IT 362467-62-7 362467-63-8 362467-64-9

(isoalloxazine derivs. to neutralize biol. microorganism contaminants
in fluids or on surfaces in relation to activation by light or pH)

RN 362467-62-7 USPATFULL

CN D-Ribitol, 1-[7-[bis(2-chloroethyl)amino]-3,4-dihydro-8-methyl-2,4-dioxobenzo[g]pteridin-10(2H)-yl]-1-deoxy- (9CI) (CA INDEX NAME)

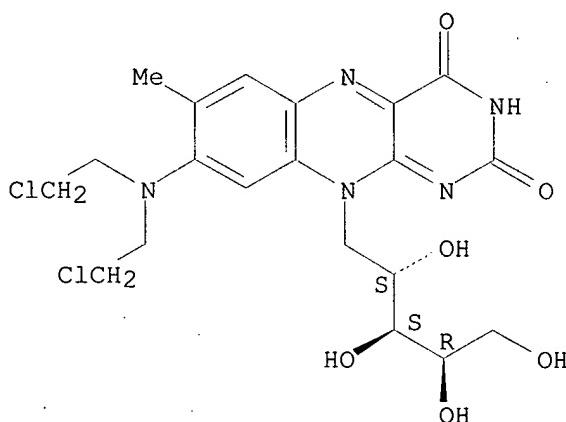
Absolute stereochemistry.



RN 362467-63-8 USPATFULL

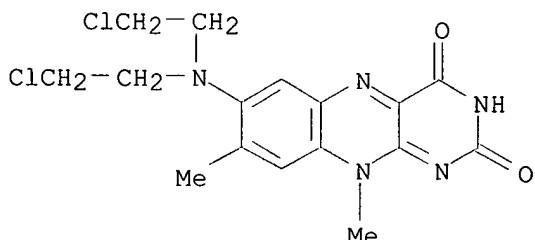
CN D-Ribitol, 1-[8-[bis(2-chloroethyl)amino]-3,4-dihydro-7-methyl-2,4-dioxobenzo[g]pteridin-10(2H)-yl]-1-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 362467-64-9 USPATFULL

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7-[bis(2-chloroethyl)amino]-8,10-dimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 72 OF 72 USPATFULL

ACCESSION NUMBER: 2001:121227 USPATFULL

TITLE: Isoalloxazine derivatives to neutralize biological contaminants

INVENTOR(S): Platz, Matthew Stewart, Columbus, OH, United States
 Goodrich, Jr., Raymond Paul, Denver, CO, United States
 PATENT ASSIGNEE(S): Gambro, Inc., Lakewood, CA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6268120	B1	20010731
APPLICATION INFO.:	US 1999-420652		19991019 (9)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Shah, Mukund J.		
ASSISTANT EXAMINER:	Liu, Hong		
LEGAL REPRESENTATIVE:	Greenlee Winner & Sullivan, P.C.		
NUMBER OF CLAIMS:	7		
EXEMPLARY CLAIM:	1		
LINE COUNT:	1217		

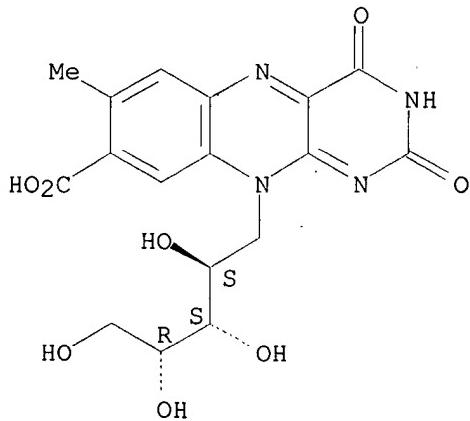
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Methods are provided for neutralization of microorganisms in fluids or on surfaces. Preferably the fluids contain blood or blood products and comprise biologically active proteins. Preferred methods include the steps of adding an activation-effective amount of a microorganism neutralizer with an isoalloxazine backbone to a fluid and exposing the fluid to a triggering event. Preferred triggering events include light of a suitable wavelength and intensity to activate the microorganism neutralizer or a pH sufficient to activate the microorganism neutralizer. Other fluids, including juices, water and the like, may also be decontaminated by these methods as may surfaces of foods, animal carcasses, wounds, food preparation surfaces and bathing and washing vessel surfaces. Compounds with an isoalloxazine backbone are also provided.

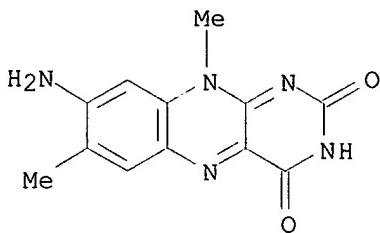
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 28083-73-0
 (neutralization of biol. contaminants by isoalloxazine derivs.)
 RN 28083-73-0 USPATFULL
 CN Riboflavin, 8-carboxy-8-demethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

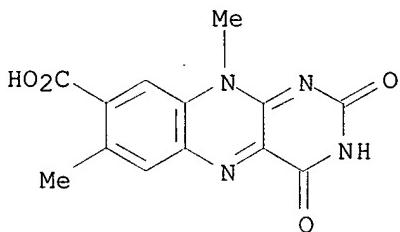


IT 3942-96-9P 101750-71-4P
 (neutralization of biol. contaminants by isoalloxazine derivs.)
 RN 3942-96-9 USPATFULL
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



RN 101750-71-4 USPATFULL

CN Benzo[g]pteridine-8-carboxylic acid, 2,3,4,10-tetrahydro-7,10-dimethyl-2,4-dioxo- (6CI, 9CI) (CA INDEX NAME)

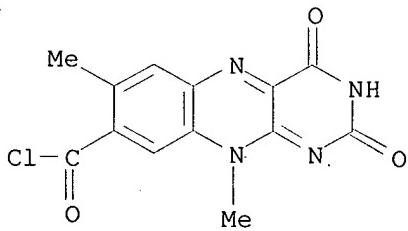


IT 335333-92-1P 335333-93-2P

(neutralization of biol. contaminants by isoalloxazine derivs.)

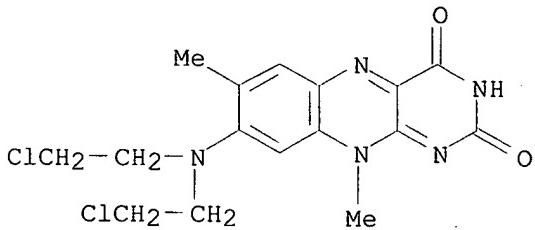
RN 335333-92-1 USPATFULL

CN Benzo[g]pteridine-8-carbonyl chloride, 2,3,4,10-tetrahydro-7,10-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



RN 335333-93-2 USPATFULL

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-[bis(2-chloroethyl)amino]-7,10-dimethyl- (9CI) (CA INDEX NAME)



IT 47061-66-5 335333-94-3 335333-95-4

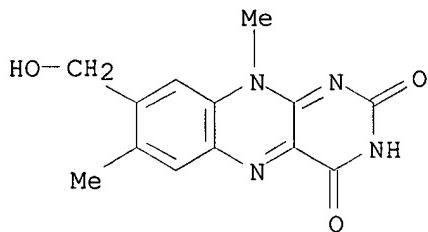
335333-96-5

(neutralization of biol. contaminants by isoalloxazine derivs.)

RN 47061-66-5 USPATFULL

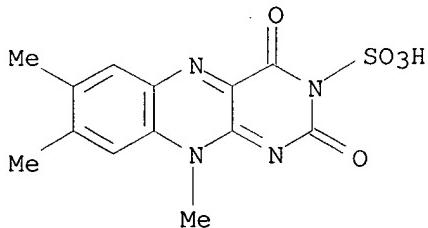
CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-(hydroxymethyl)-7,10-dimethyl-

(9CI) (CA INDEX NAME)



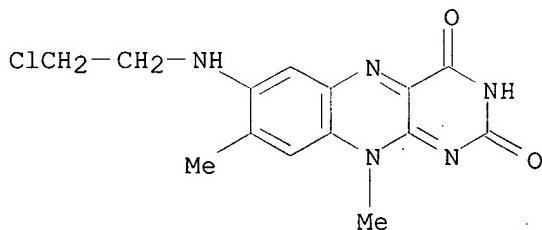
RN 335333-94-3 USPATFULL

CN Benzo[g]pteridine-3(2H)-sulfonic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



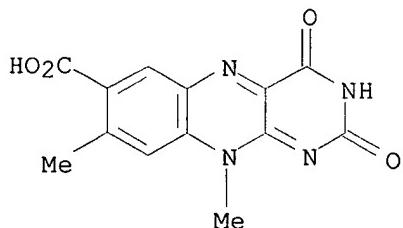
RN 335333-95-4 USPATFULL

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7-[(2-chloroethyl)amino]-8,10-dimethyl- (9CI) (CA INDEX NAME)



RN 335333-96-5 USPATFULL

CN Benzo[g]pteridine-7-carboxylic acid, 2,3,4,10-tetrahydro-8,10-dimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



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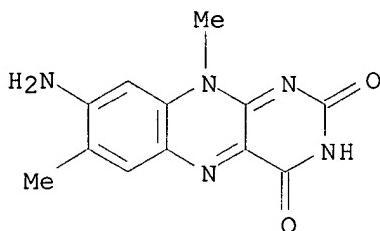
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          71-00-1/BI OR 73-22-3/BI OR 73-24-5/BI OR 9000-94-6/BI OR
          9001-26-7/BI OR 9001-28-9/BI OR 9001-29-0/BI OR 9001-30-3/BI
          OR 9002-01-1/BI OR 9002-72-6/BI OR 9013-55-2/BI OR 9031-37-2/BI
          OR 9035-81-8/BI OR 9038-70-4/BI OR 9055-02-1/BI OR 98-92-0/BI
          OR 101750-71-4/BI OR 113189-02-9/BI OR 28083-73-0/BI OR
          335333-92-1/BI OR 335333-93-2/BI OR 335333-94-3/BI OR 335333-95
          -4/BI OR 335333-96-5/BI OR 362467-62-7/BI OR 362467-63-8/BI OR
          362467-64-9/BI OR 3942-96-9/BI OR 47061-66-5/BI OR 616-91-1/BI
          OR 9001-27-8/BI)
L6      12 SEA FILE=REGISTRY ABB=ON L5 AND NR>2
L11     STR
L13     4344 SEA FILE=REGISTRY SSS FUL L11
L19     STR
L24     STR
L26     76 SEA FILE=REGISTRY SUB=L13 SSS FUL (L19 OR L24)
L30     STR
L32     43 SEA FILE=REGISTRY SUB=L26 SSS FUL (L11 NOT L30)
L36     7 SEA FILE=CAOLD ABB=ON L6 OR L32
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>>> d iall hitstr l36 1-7; fil hom

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L36 ANSWER 1 OF 7 CAOLD COPYRIGHT 2002 ACS
ACCESSION NUMBER: CA63:16352d CAOLD
TITLE: acenaphthazine
AUTHOR NAME: Schoenberg, Alexander; Singer, E.
INDEX TERM: 207-04-5 3942-95-8 3942-96-9 4089-83-2
             4098-37-7
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IT 3942-96-9
RN 3942-96-9 CAOLD
CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA
INDEX NAME)
```



L36 ANSWER 2 OF 7 CAOLD COPYRIGHT 2002 ACS

ACCESSION NUMBER: CA61:15025h CAOLD

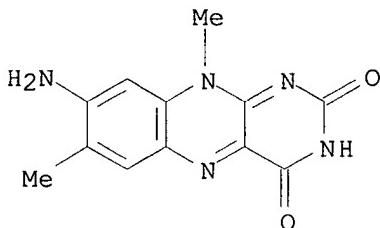
TITLE: microbiol. and enzymic assays of riboflavin analogs

AUTHOR NAME: Yang, Chung Shu; Arsenis, C.; McCormick, D. B.

INDEX TERM: 303-59-3 303-66-2 **3942-96-9** 4430-73-3
5618-55-3 5618-80-4 5618-81-5 5618-82-6 5618-83-7
5618-90-6 5618-91-7 5648-97-5 5720-12-7 98693-47-1
98855-16-4 106861-29-4IT **3942-96-9**

RN 3942-96-9 CAOLD

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



L36 ANSWER 3 OF 7 CAOLD COPYRIGHT 2002 ACS

ACCESSION NUMBER: CA61:9498g CAOLD

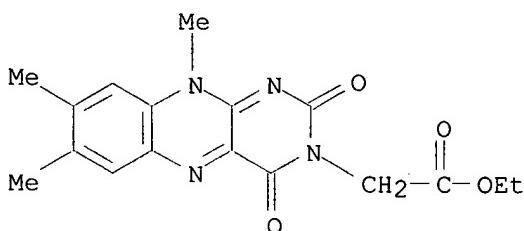
TITLE: flavine series - (IX) spectra and structures of the species concerned in the flavine redox system

AUTHOR NAME: Dudley, Kenneth H.; Ehrenberg, A.; Hemmerich, P.; Mueller, F.

INDEX TERM: 752-13-6 1214-95-5 4074-58-2 4098-37-7 4250-90-2
13345-95-4 13641-12-8 13858-04-3 14453-92-0 14453-93-1
14453-95-3 14453-97-5 14454-00-3 14454-04-7 14454-09-2
14454-10-5 14471-76-2 18717-85-6 18950-64-6 25431-13-4
26257-55-6 33174-44-6 35835-02-0 39092-09-6 58017-92-8
64135-79-1 **74178-39-5** 82019-34-9 91803-43-9
91974-67-3 91974-68-4 94350-74-0 94350-75-1 96078-53-4
96229-87-7 98074-49-8 98074-50-1 98148-00-6 98309-56-9
98764-35-3 101522-23-0 101764-26-5 104158-90-9 104718-59-4
106217-12-3 106384-79-6IT **74178-39-5**

RN 74178-39-5 CAOLD

CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (7CI, 9CI) (CA INDEX NAME)



L36 ANSWER 4 OF 7 CAOLD COPYRIGHT 2002 ACS

ACCESSION NUMBER: CA60:14780f CAOLD

TITLE: kinetics of histaminase

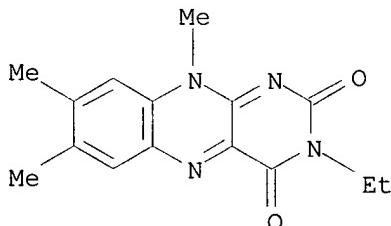
AUTHOR NAME: Morrison, George A.

INDEX TERM: 14684-43-6 18636-32-3 20227-26-3 20469-92-5
74178-39-5

IT 20469-92-5 74178-39-5

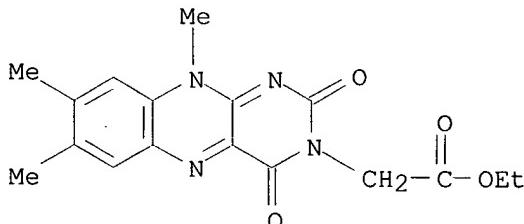
RN 20469-92-5 CAOLD

CN Lumazine, 3-ethyl- (8CI) (CA INDEX NAME)



RN 74178-39-5 CAOLD

CN Benzo[g]pteridine-3(2H)-acetic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, ethyl ester (7CI, 9CI) (CA INDEX NAME)



L36 ANSWER 5 OF 7 CAOLD COPYRIGHT 2002 ACS

ACCESSION NUMBER: CA54:18534h CAOLD

TITLE: lumiflavine series - (VI) alkylation and dealkylation reactions with isoalloxazines-1,3,10-trimethylflavosemiquinone

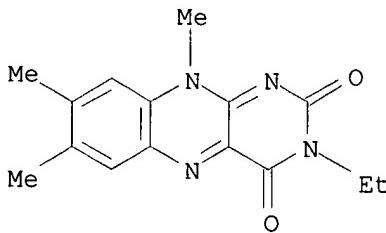
AUTHOR NAME: Hemmerich, Peter; Prijs, B.; Erlenmeyer, H.

INDEX TERM: 1086-80-2 2962-90-5 4074-59-3 14684-48-1 15989-59-0
15989-60-3 15989-61-4 18636-32-3 20469-92-5
26257-55-6 33174-44-6 58017-93-9 72184-50-0 97061-90-0
106275-40-5 109016-96-8 109472-67-5 109535-99-1 109731-52-4
109845-90-1 109940-88-7 111296-39-0 111616-92-3 117000-81-4
121761-06-6

IT 20469-92-5

RN 20469-92-5 CAOLD

CN Lumazine, 3-ethyl- (8CI) (CA INDEX NAME)



L36 ANSWER 6 OF 7 CAOLD COPYRIGHT 2002 ACS

ACCESSION NUMBER: CA54:18533c CAOLD

TITLE: lumiflavine series - (V) specific reactivity of
8-substituents in the isoalloxazine nucleus-flavine dimers

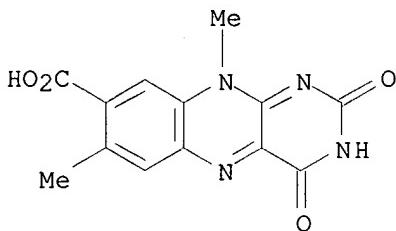
AUTHOR NAME: Hemmerich, Peter; Prijs, B.; Erlenmeyer, H.

INDEX TERM: 4098-37-7 5618-84-8 15436-36-9 21652-23-3 22525-78-6
84869-39-6 96323-42-1 **101750-71-4** 102948-83-4
119079-36-6 119079-37-7 119716-95-9 122148-00-9 122211-83-0
122215-53-6

IT **101750-71-4**

RN 101750-71-4 CAOLD

CN Benzo[g]pteridine-8-carboxylic acid, 2,3,4,10-tetrahydro-7,10-dimethyl-2,4-dioxo- (6CI, 9CI) (CA INDEX NAME)



L36 ANSWER 7 OF 7 CAOLD COPYRIGHT 2002 ACS

ACCESSION NUMBER: CA54:4602i CAOLD

TITLE: lumiflavine series - (IV)

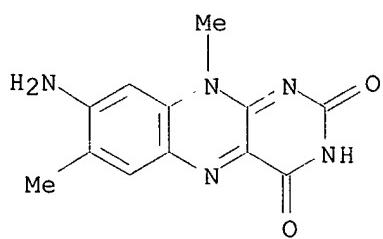
AUTHOR NAME: Hemmerich, Peter; Prijs, B.; Erlenmeyer, H.

INDEX TERM: 1088-56-8 **3942-96-9** 4098-37-7 64713-17-3
72184-50-0 97881-26-0 98110-33-9 99989-88-5 100708-47-2
102880-91-1 108487-15-6 108696-24-8 109128-13-4 109163-18-0
109448-83-1 109448-84-2 109448-94-4 109448-95-5 110030-87-0
110206-76-3 111358-20-4 113040-05-4 114930-33-5 114930-34-6
117026-33-2 118803-44-4 119530-76-6 131977-20-3

IT **3942-96-9**

RN 3942-96-9 CAOLD

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



FILE 'HOME' ENTERED AT 14:21:11 ON 13 MAR 2002

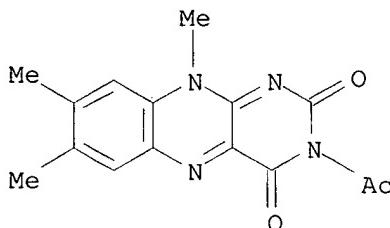
AB Monochlorophosphoric acid was used for selective 5'-monophosphorylation of riboflavin and derivs. This reaction yields invariably up to 20% of an isomer, which was sepd. by preparative thick-layer chromatog. and shown to be the 4'-monophosphate. Base catalysis of FMN does not yield 2',3',4'-triacetylflavine mononucleotide as claimed by E. D. Khomutova, et al. (1965), but up to 80% 2',3'-diacetylflavine 4',5'-cyclophosphate as the main product, which is stable under neutral and weak acidic conditions and does not hydrolyze to 2',3'-diacetylflavine 5'-monophosphate as claimed by D. B. McCormick (1974). The various flavine phosphates and their acetyl derivs. were identified by pH-titrn., electrophoresis, and PMR spectrometry which permit direct analyses of crude reaction products as well as a rapidly purity check of com. FMN.

IT 60823-53-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 60823-53-2 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 3-acetyl-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 53 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:495986 CAPLUS

DOCUMENT NUMBER: 83:95986

TITLE: Excited-state reactions of oxidized flavine derivatives

AUTHOR(S): Lasser, Nehama; Feitelson, Jehuda

CORPORATE SOURCE: Dep. Phys. Chem., Hebrew Univ., Jerusalem, Israel

SOURCE: Photochem. Photobiol. (1975), 21(4), 249-54

CODEN: PHCBAP

DOCUMENT TYPE: Journal

LANGUAGE: English

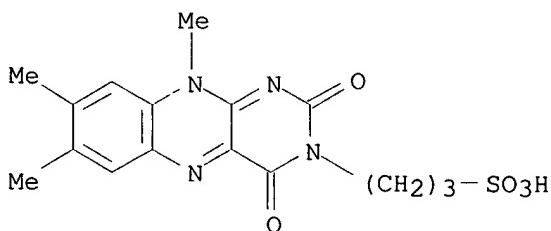
AB The reactivity of flavine mononucleotide and lumiflavine triplets was studied by flash and laser photolysis. The rate consts. of the triplets with O₂, with flavine ground-state mols. and with Br⁻ ions were detd. Although in soln. at room temp., the protonated flavin triplet, 3FlH⁺, is not formed directly from its very short lived singlet state, a transient, which results from protonation of the neutral triplet is believed to be 3FlH⁺. This conclusion is based on a comparison between the neutral and the protonated triplet spectra in a low-temp. glass. The protonated triplet may also be formed by sensitization via the phenanthrene triplet.

IT 56502-48-8

RL: RCT (Reactant)
(photolysis of)

RN 56502-48-8 CAPLUS

CN Benzo[g]pteridine-3(2H)-propanesulfonic acid, 4,10-dihydro-7,8,10-trimethyl-2,4-dioxo-, barium salt (9CI) (CA INDEX NAME)



● 1/2 Ba

L37 ANSWER 54 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:90551 CAPLUS

DOCUMENT NUMBER: 84:90551

TITLE: Inter- and intramolecular effects of tyrosyl residues on flavine triplets and radicals as investigated by flash photolysis

AUTHOR(S): McCormick, Donald B.; Falk, Michael C.; Rizzuto, Frank; Tollin, Gordon

CORPORATE SOURCE: Sect. Biochem., Cornell Univ., Ithaca, N. Y., USA

SOURCE: Photochem. Photobiol. (1975), 22(5), 175-81

CODEN: PHCBAP

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Addn. of tyrosine and its derivs. to aq. solns. of flavines did not significantly hinder formation of the flavine triplet or the rate of oxidn. of the flavine radical produced by reaction of the triplet with the Ph residue but the rate of radical decay was decreased. The main photochem. reaction is formation of the phenoxy-type radicals which do not participate in flavine radical decay in competition with O. Intramol. complexed flavines, e.g. N10-flavanyl O-methyltyrosine, exhibited 1st order radical decay, reflecting the reverse electron transfer between phenoxy and flavine radicals. The tyrosyl group within the active site of mitochondrial monoamine oxidase is not easily photooxidized by the 8.alpha.- (S-L-cysteinyl)flavine involved, since the thioether bond reduces triplet prodn. On oxidn. of the thioether to sulfone, the triplet yield is partially restored and flavine radicals may be generated from the intramol. or an intermol. tyrosyl group.

IT 20806-70-6

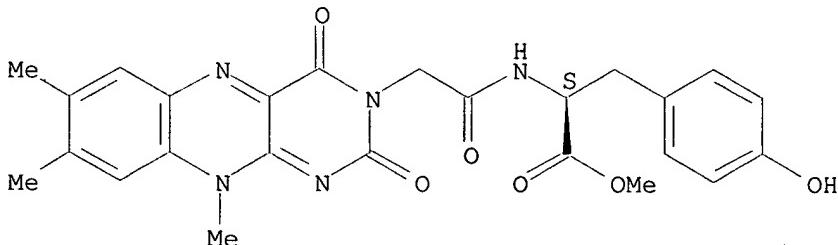
RL: RCT (Reactant)

(flash photolysis of aq. solns. of, in presence of tyrosine ester)

RN 20806-70-6 CAPLUS

CN L-Tyrosine, N-[(4,10-dihydro-7,8,10-trimethyl-2,4-dioxobenzo[g]pteridin-3(2H)-yl)acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



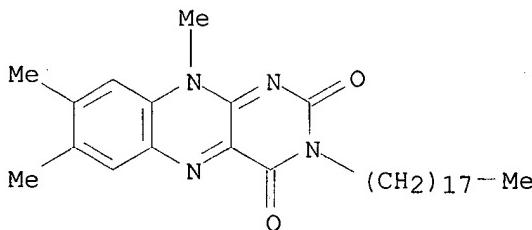
L37 ANSWER 55 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1975:403042 CAPLUS
 DOCUMENT NUMBER: 83:3042
 TITLE: Fluorescence polarization in a planar array of pigment molecules. Theoretical treatment and application to flavins incorporated into artificial membranes
 AUTHOR(S): Frehland, E.; Trissl, H. W.
 CORPORATE SOURCE: Dep. Phys., Univ. Konstanz, Constance, Ger.
 SOURCE: J. Membr. Biol. (1975), 21(1-2), 147-73
 CODEN: JMBBBO
 DOCUMENT TYPE: Journal
 LANGUAGE: English.

AB A quant. fluorescence polarization theory of mols. bound to 2-dimensional plane layers was developed for when the electronic transition moments of absorption and emission are parallel within the fluorescent mols. The transition moments are assumed to be in preferred orientation with respect to the normal to the plane and to be randomly oriented within the plane (rotational symmetry with the normal as axis of symmetry). Three basic model distributions of transition moments were investigated quant. These model distributions represent a simplification but in most cases may be expected to describe reality with sufficient accuracy. For all distributions, 2 cases of different mobility of mols. were treated: (a) the lifetime of fluorescence is small compared with the characteristic relaxation time of the distribution, and (b) the lifetime of fluorescence is long, so that a complete reorientation of transition moments during the excited state can take place. From the quant. calcns., 4 characteristic quantities were derived, which are appropriate for the anal. of exptl. data. Expts. were carried out with phosphatidylcholine bilayer membranes which contain 3 differently substituted amphiphilic flavines [7, 8, 10-trimethyl-3-octadecylisoalloxazine, 3, 7, 8-trimethyl-10-[2-(octadec[9c]enoxy)ethyl]isoalloxazine, and 3-methyl-10-octadecylisoalloxazine]. All 3 flavines yielded similar data. Their analyses predict free and fast mobility of the flavine chromophore.

IT 53965-14-3

RL: BIOL (Biological study)
(fluorescence polarization of lecithin membrane-bound)

RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
(CA INDEX NAME)

L37 ANSWER 56 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1976:12986 CAPLUS
 DOCUMENT NUMBER: 84:12986
 TITLE: Analogs of riboflavin, lumiflavin, and alloxazine derivatives. I. Effect of analogs on the synthesis of riboflavin and growth of *Bacillus subtilis*
 AUTHOR(S): Stepanov, A. I.; Tul'chinskaya, L. S.; Berezovskii, V. M.; Kukanova, A. Ya.
 CORPORATE SOURCE: Inst. Genet. Sel. Ind. Microorg., Moscow, USSR

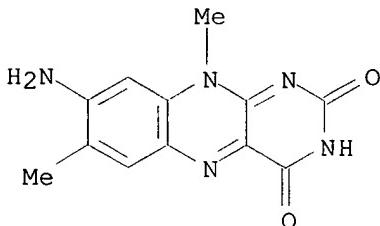
SOURCE: Genetika (1975), 11(9), 116-24
 CODEN: GNKAA5

DOCUMENT TYPE: Journal
 LANGUAGE: Russian

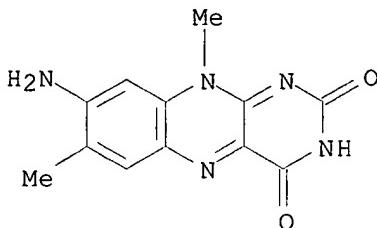
AB The effect of 44 analogs of riboflavin [83-88-5] and lumiflavin [1088-56-8], and derivs. of alloxazine [490-59-5] was studied on 3 strains of *B. subtilis* with various capacities for synthesis of vitamin B2 and different genetic states of the riboflavin operon. The relation between structure and activity is discussed.

IT 3942-96-9
 RL: PRP (Properties)
 (Bacillus subtilis growth and riboflavin formation response to)

RN 3942-96-9 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 57 OF 72 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1974:121235 CAPLUS
 DOCUMENT NUMBER: 80:121235
 TITLE: Allo- and isoalloxazines. XXXVI. Effect of different substituents on the redox properties of derivatives of riboflavin and related compounds
 AUTHOR(S): Tul'chinskaya, L. S.; Zhilina, T. A.; Berezovskii, V. M.
 CORPORATE SOURCE: Vses. Nauchno-Issled. Vitam. Inst., Moscow, USSR
 SOURCE: Zh. Obshch. Khim. (1974), 44(2), 406-10
 CODEN: ZOKHA4
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI For diagram(s), see printed CA Issue.
 AB The effect of substituents on the redox potentials of isoalloxazines (I; R = H, Me, R1 = H, Me, Cl, NH2, OH, Br, ribitylamino, R2 = ribityl, tetraacetylribityl, Me, glucityl) and alloxazines (II; R3 = H, Br, R4 = H, Me, NH2, R5 = H, NH2, NMe2, Cl, Br, OH, Me, R6 = H, NH2, Br) were detd. Redox potentials increased when NH2, OH, Cl, Br were substituted in the 8 position (R, R5) compared to the corresponding values for the 7 position (R1, R4).
 IT 3942-96-9
 RL: PRP (Properties)
 (oxidn.-redn. potential of)
 RN 3942-96-9 CAPLUS
 CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 58 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:53065 CAPLUS

DOCUMENT NUMBER: 82:53065

TITLE: Incorporation of fluorescent pigments into bilayer membranes

AUTHOR(S): Trissl, H. W.

CORPORATE SOURCE: Dep. Biol., Univ. Konstanz, Constance, Ger.

SOURCE: Biochim. Biophys. Acta (1974), 367(3), 326-37

CODEN: BBACAO

DOCUMENT TYPE: Journal

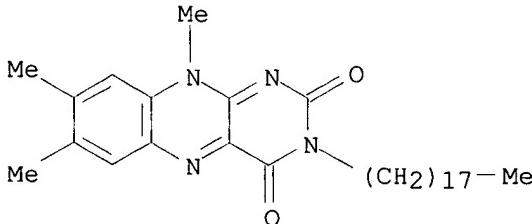
LANGUAGE: English

AB A technique was developed which is appropriate for quant. fluorescence anal. of pigments in artificial lipid bilayer membranes. The technique is based on taking a monochromatic picture of the point where a parallel light beam crosses the membrane. The d. of the neg. can be used as a std. for the fluorescence intensity. A calibration curve is obtained by substituting the membrane with an optical microcell filled with solns. of the examd. pigment. Thus, a continuous observation is possible. The abs. sensitivity of the technique is given. The incorporation of rubrene, Mg octaethylporphyrin, and 3 amphiphilic flavines, substituted with long hydrocarbon chains, into bilayer membranes was investigated. If identical concns. of these pigments were added to the membrane-forming soln., vast differences in the membrane concns. were found. The amt. of incorporated pigment also depended on the kind of lipid as well as the lipid prepns. The expts. with the amphiphilic flavines indicated that the hydrophilic flavine nucleus is situated in the membrane/H₂O interface, whereas the hydrophobic hydrocarbon chain sticks into the lipophilic interior of the bilayer.

IT 53965-14-3

RL: PROC (Process)
(lipid bilayer membrane incorporation of)

RN 53965-14-3 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 7,8,10-trimethyl-3-octadecyl- (9CI)
(CA INDEX NAME)

L37 ANSWER 59 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1974:3469 CAPLUS

DOCUMENT NUMBER: 80:3469

TITLE: Substitution and addition reactions in the alloxazine

AUTHOR(S): and isoalloxazine series
 Aksel'rod, Zh. I.; Berezovskii, V. M.
 CORPORATE SOURCE: USSR
 SOURCE: Vitam. Vitam. Prep. (1973), 92-111. Editor(s):
 Yakovlev, V. A. "Meditina": Moscow, USSR.
 CODEN: 27GWA7

DOCUMENT TYPE: Conference
 LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

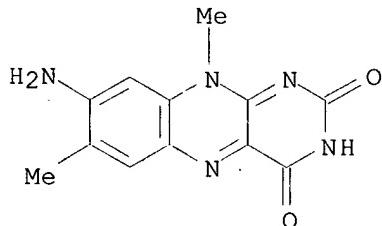
AB Fluorescence spectra were detd. for alloxazines (I; R = H, Me, Cl, SO₂NH₂, NH₂, AcNH, BzNH, p-MeC₆H₄SO₂; R₁ = H, Me, Cl), II (R = H, Me; R₁ = H, Bz, Ac, p-MeC₆H₄SO₂), isoalloxazines (III; R = Me, ribityl; R₁ = Me, Cl, NH₂), and 20 addnl. substituted derivs. prepd. by known methods.

IT 3942-96-9

RL: PRP (Properties)
 (ir spectrum of)

RN 3942-96-9 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)



L37 ANSWER 60 OF 72 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1972:419609 CAPLUS

DOCUMENT NUMBER: 77:19609

TITLE: Allo- and isoalloxazines. XXXI. Synthesis of hydroxy analogs of natural flavines

AUTHOR(S): Polyakova, N. A.; Tul'chinskaya, L. S.; Zapesochnaya, L. G.; Berezovskii, V. M.

CORPORATE SOURCE: Vses. Nauchno-Issled. Vitam. Inst., Moscow, USSR

SOURCE: Zh. Obshch. Khim. (1972), 42(2), 465-8

CODEN: ZOKHA4

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Diazotization of 7-aminoalloxazine in 70% H₂SO₄ followed by diln. and heating finally at reflux 1 hr gave 7-hydroxyalloxazine. Similarly was prepd. 7-hydroxy(nor)lumichrome; 7-hydroxy(nor)lumiflavine; and 7-hydroxy(nor)riboflavine. The absorption spectra of these showed that introduction of HO or NH₂ groups into the 7-position in the isoalloxazine ring system results in a similar electron donor contribution to the electron system; this is not the case for the alloxazine ring system. The above 7-hydroxyalloxazines have a high level of electrophilic substitution reactivity and like phenols can azo couple with diazotized amines.

IT 3942-96-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 3942-96-9 CAPLUS

CN Benzo[g]pteridine-2,4(3H,10H)-dione, 8-amino-7,10-dimethyl- (9CI) (CA INDEX NAME)